

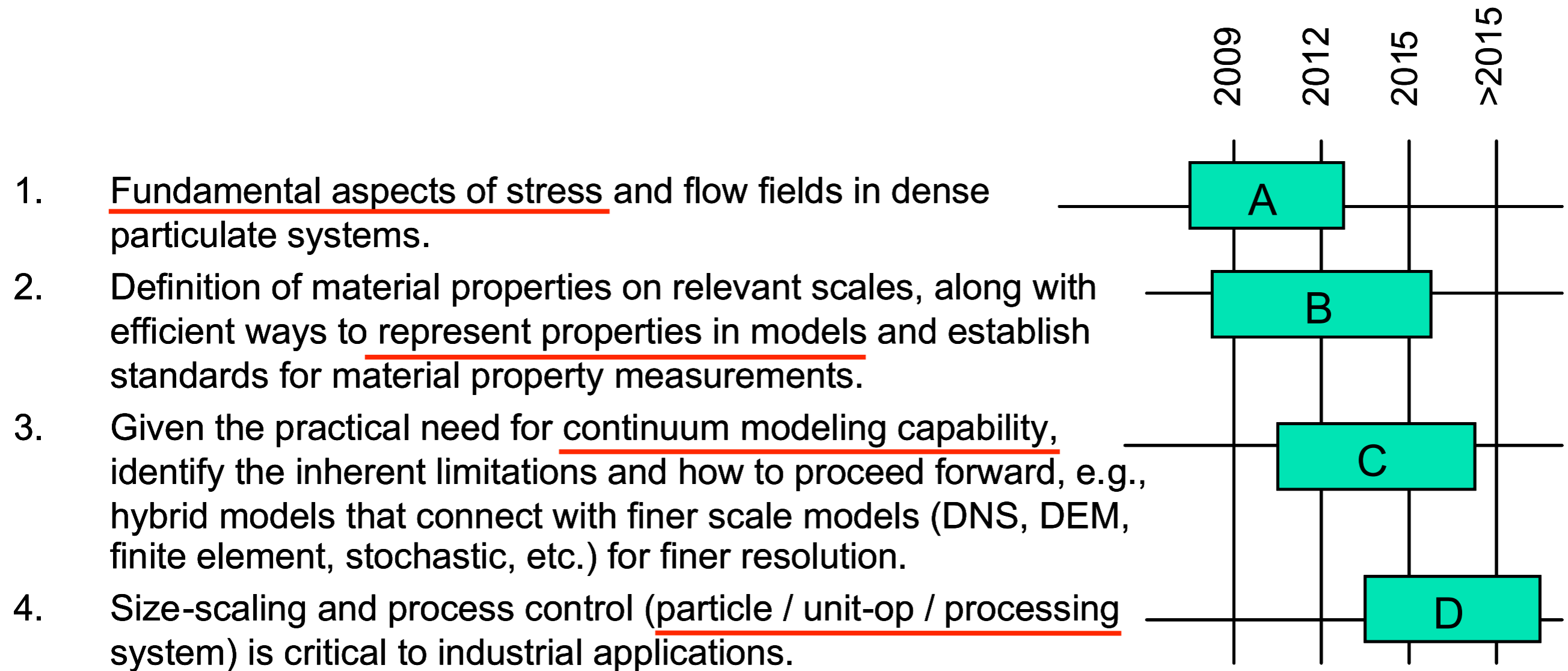
# Granular Rheology in the Quasi-static, Intermediate and Rapid Flow Regimes: Towards a Comprehensive Model

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Department of Chemical Engineering  
Princeton University

NETL Workshop on Multiphase Flow Science  
Pittsburgh, PA  
May 4, 2010



# Roadmap for dense granular flow

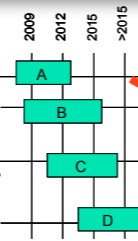


# Connection to roadmap



Key questions addressed:

1. Fundamental aspects of stress and flow fields in dense particulate systems.
2. Definition of material properties on relevant scales, along with efficient ways to represent properties in models and establish standards for material property measurements.
3. Given the practical need for continuum modeling capability, identify the inherent limitations and how to proceed forward, e.g., hybrid models that connect with finer scale models (DNS, DEM, finite element, stochastic, etc.) for finer resolution.
4. Size-scaling and process control (particle / unit-op / processing system) is critical to industrial applications.



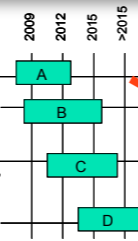
Action taken in our project:

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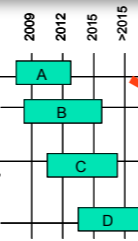
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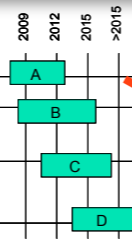
- What defines the stress in quasi-static regime?
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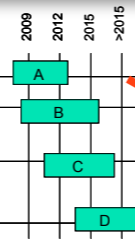
- What defines the stress in quasi-static regime?
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- Continuum rheological models from quasi-static to rapid flow regimes? (**Goal II in our project**)
- Identified internal variables defining stress states.
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- Developed a plasticity model for the quasi-static regime and extending to intermediate regime.

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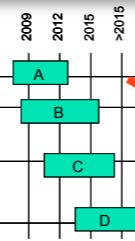
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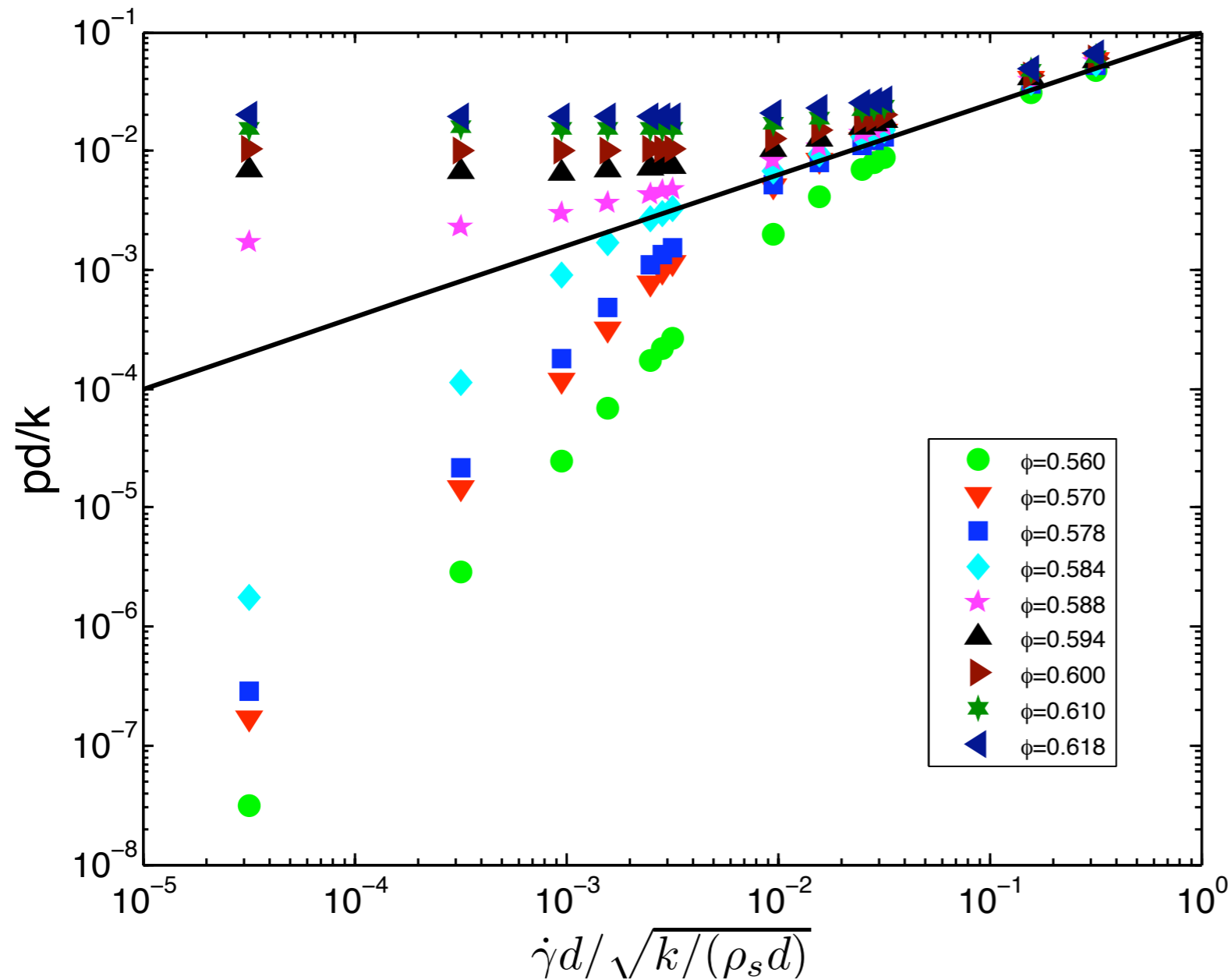


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# Flow map

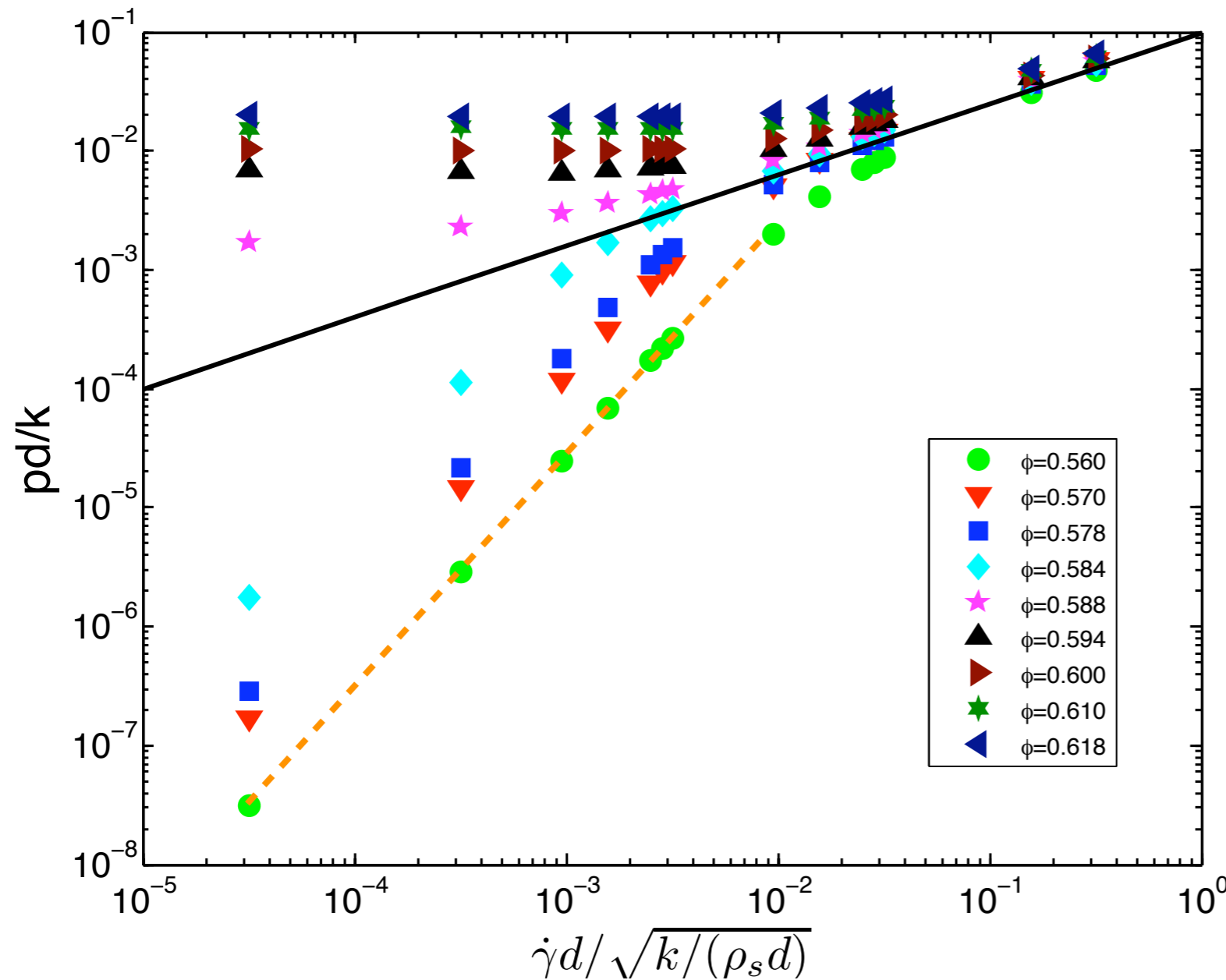


Scaled pressure  
versus scaled  
shear rate from  
steady simple  
shear simulations

$$\mu = 0.5$$

- Critical volume fraction distinguishes flow regimes and is related to jamming transition.
- Flow behaviors merge into the same scaling at high shear rates. 4 / 23

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# Outline



- Introduction to the quasi-static constitutive model
- Model calibration for a wide range of particle friction coefficients
- Extension to predict normal stress difference
- Application to hopper flows
- Rate-dependent flow behaviors
- Future work

# Model construction



- Simulate particle dynamics of homogeneous assemblies under isotropic compression or simple shear using discrete element method (DEM).
- Extract stress and structural information by averaging; seek constitutive relations.

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$$\sigma = \frac{1}{V} \sum_i^N \left[ m_i \mathbf{C}_i \mathbf{C}_i + \sum_{j, j \neq i} \frac{1}{2} \mathbf{r}_{ij} \mathbf{F}_{ij} \right]$$

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- **Coordination number**: average number of contacting neighbors

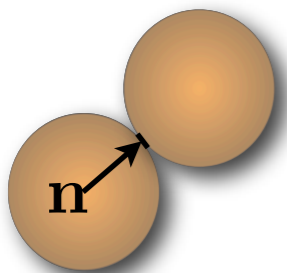
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- **Coordination number**: average number of contacting neighbors
- **Fabric tensor**: average of tensor product of unit contact normals



$$\mathbf{A} = \frac{1}{N_{c2}} \sum_{n=1}^N \sum_{c=1}^{c_p \geq 2} \mathbf{n}_{p,c} \mathbf{n}_{p,c} - \frac{1}{3} \mathbf{I}$$

# Stress model\* and closures



$$\boldsymbol{\sigma} = p\mathbf{I} - p\eta \frac{\mathbf{S}}{|\mathbf{D}|} \quad |\mathbf{D}| = \sqrt{\frac{1}{2} \mathbf{D}^T : \mathbf{D}}$$

\* D.G. Schaeffer. *J. Differ. Equ.* 66, 19, 1987; J.D. Goddard. *J. Fluid Mech.* 568, 1, 2006

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S ← Deviatoric strain rate  
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Pressure equation  $pd/k = (a_1 + a_2|A|)(Z - Z_c)^2$

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$$\sigma = \underset{\substack{\uparrow \\ \text{Pressure}}}{p} \mathbf{I} - \underset{\substack{\uparrow \\ \text{Macro-friction}}}{p\eta} \frac{\mathbf{S}}{|\mathbf{D}|}$$

$\mathbf{S} \leftarrow$  Deviatoric strain rate

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Pressure equation  $p d/k = (a_1 + a_2 |A|)(Z - Z_c)^2$

Macroscopic friction  $\eta = b_1 + b_2 \frac{A : S}{|\mathbf{D}|}$

linked to microstructure variables

# Evolution equations



## Fabric tensor

$$\dot{A} = c_1 S + c_2 |D| A + c_3 (A : D) A$$

Jaumann derivative  $\dot{A} = \frac{dA}{dt} + A \cdot W - W \cdot A$

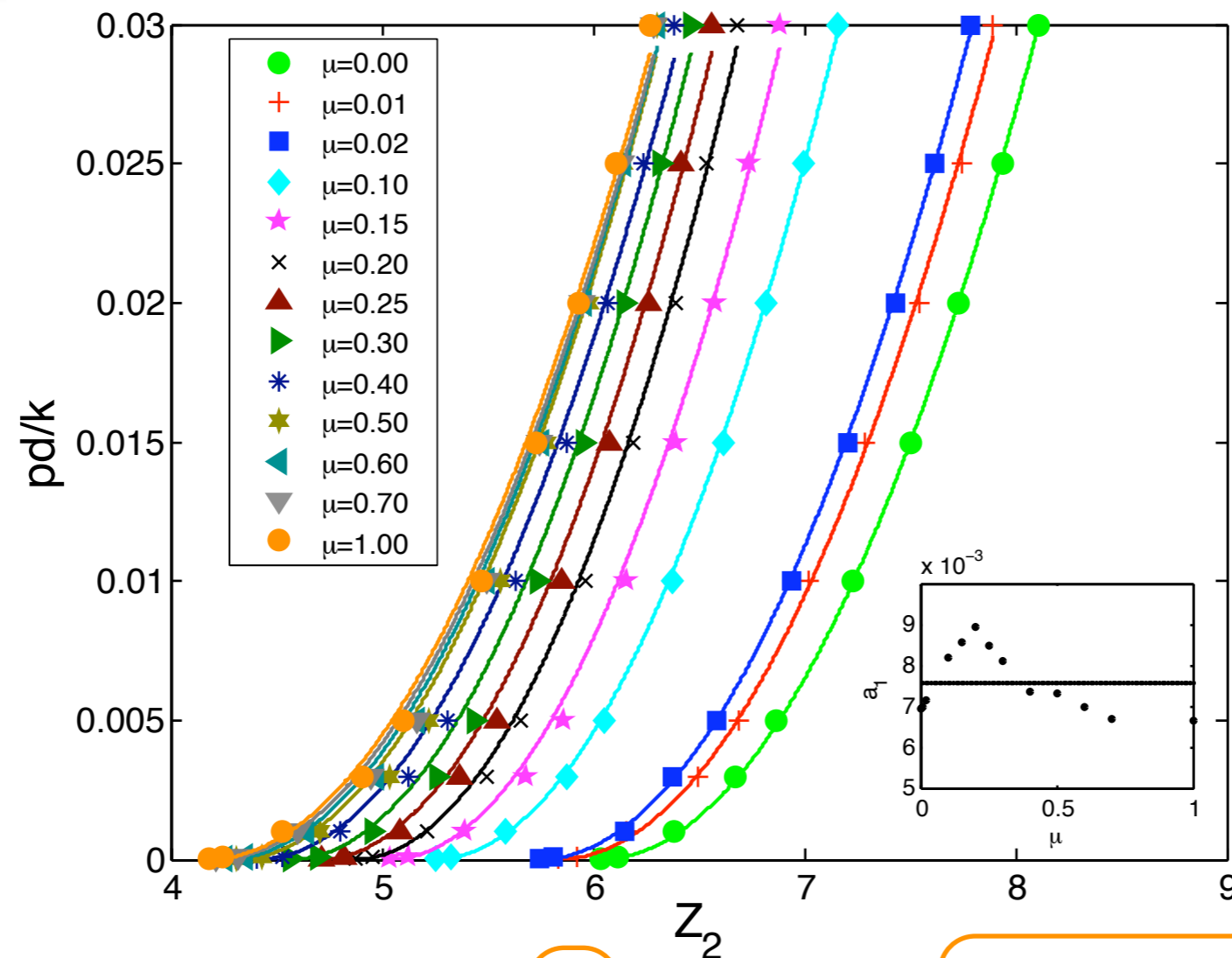
## Coordination number

$$\dot{Z} = d_1 (A : D + \chi) + d_2 |D| (f(\phi) - Z) + d_3 \text{tr}(D) \quad \dot{Z} = \frac{dZ}{dt}$$

$$\chi = (c_2 + \sqrt{c_2^2 - 8c_1 c_3}) / 2c_3$$

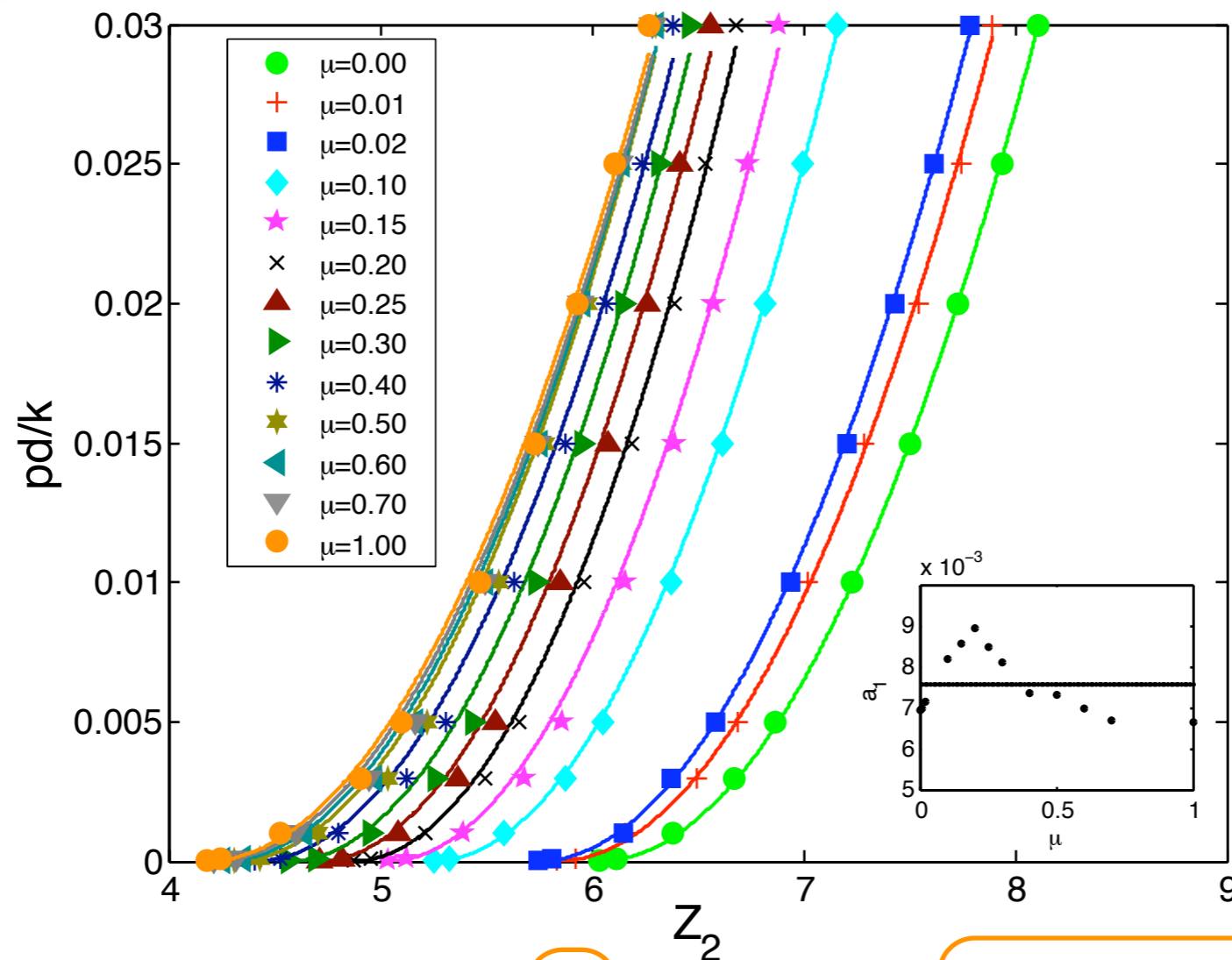
The model has been verified to be able to correctly predict complex rheological behaviors during steady and unsteady flows.

# Incorporating particle friction: isotropic compression



$$pd/k = (a_1 + a_2|A|)(Z - Z_c)^2$$

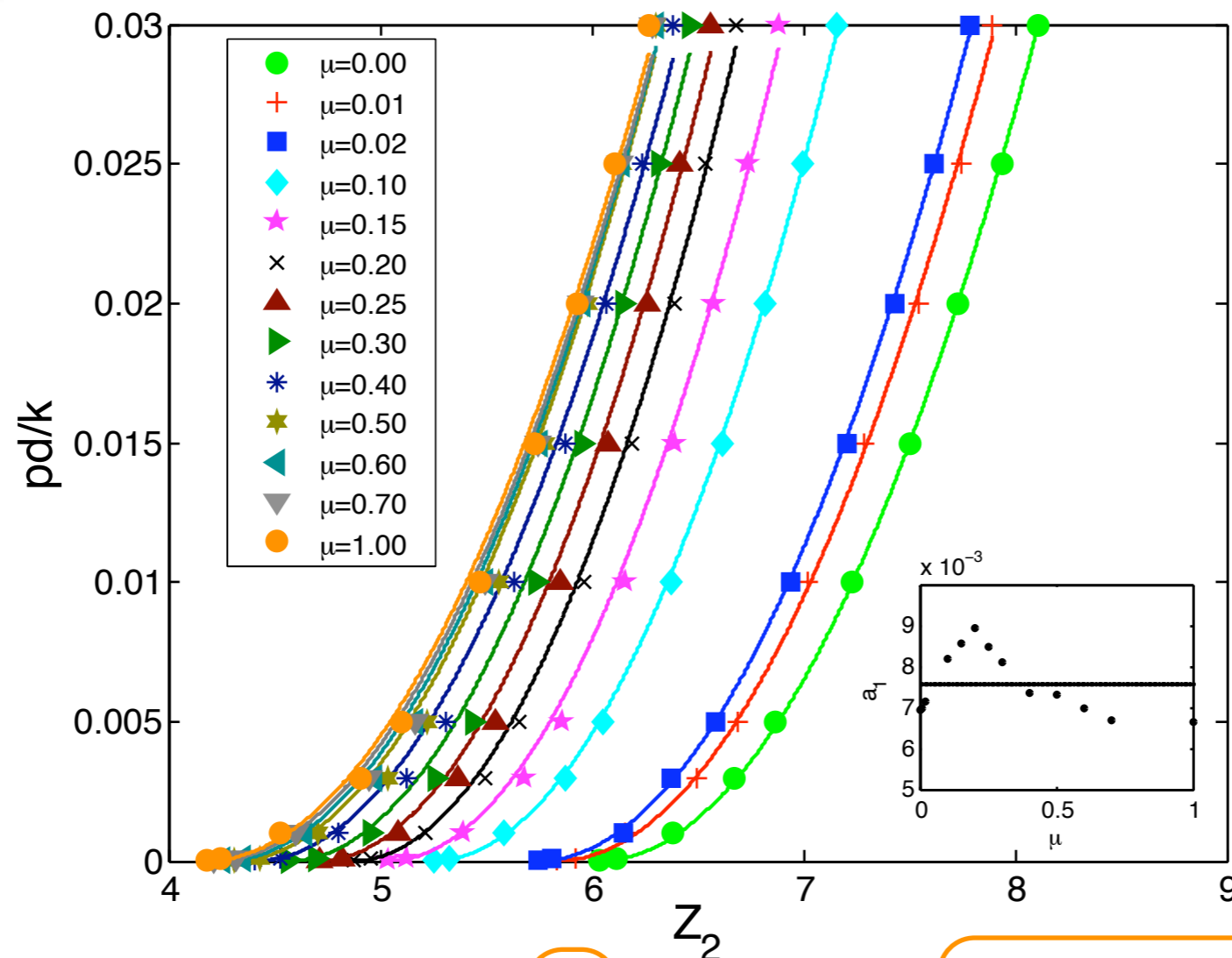
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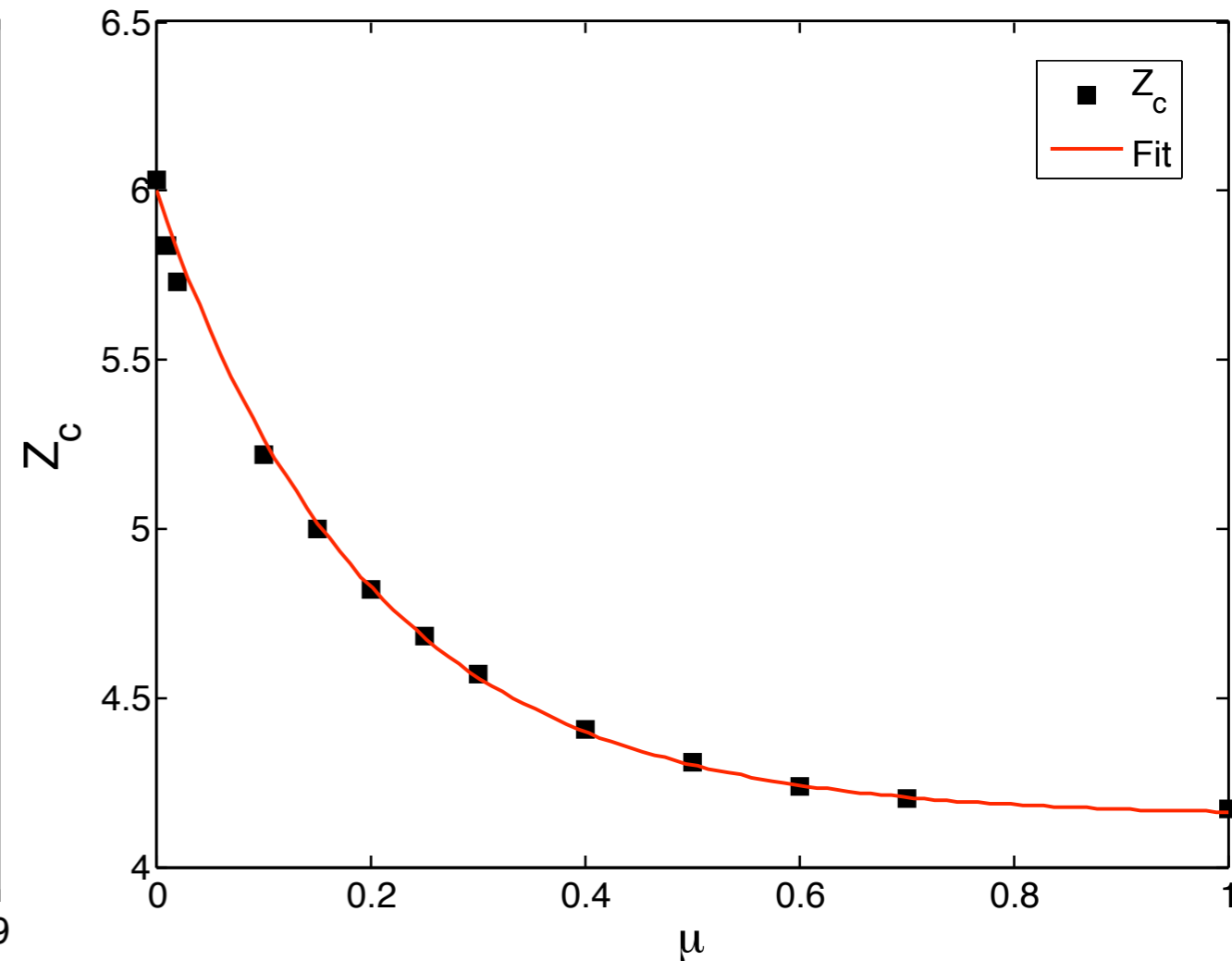
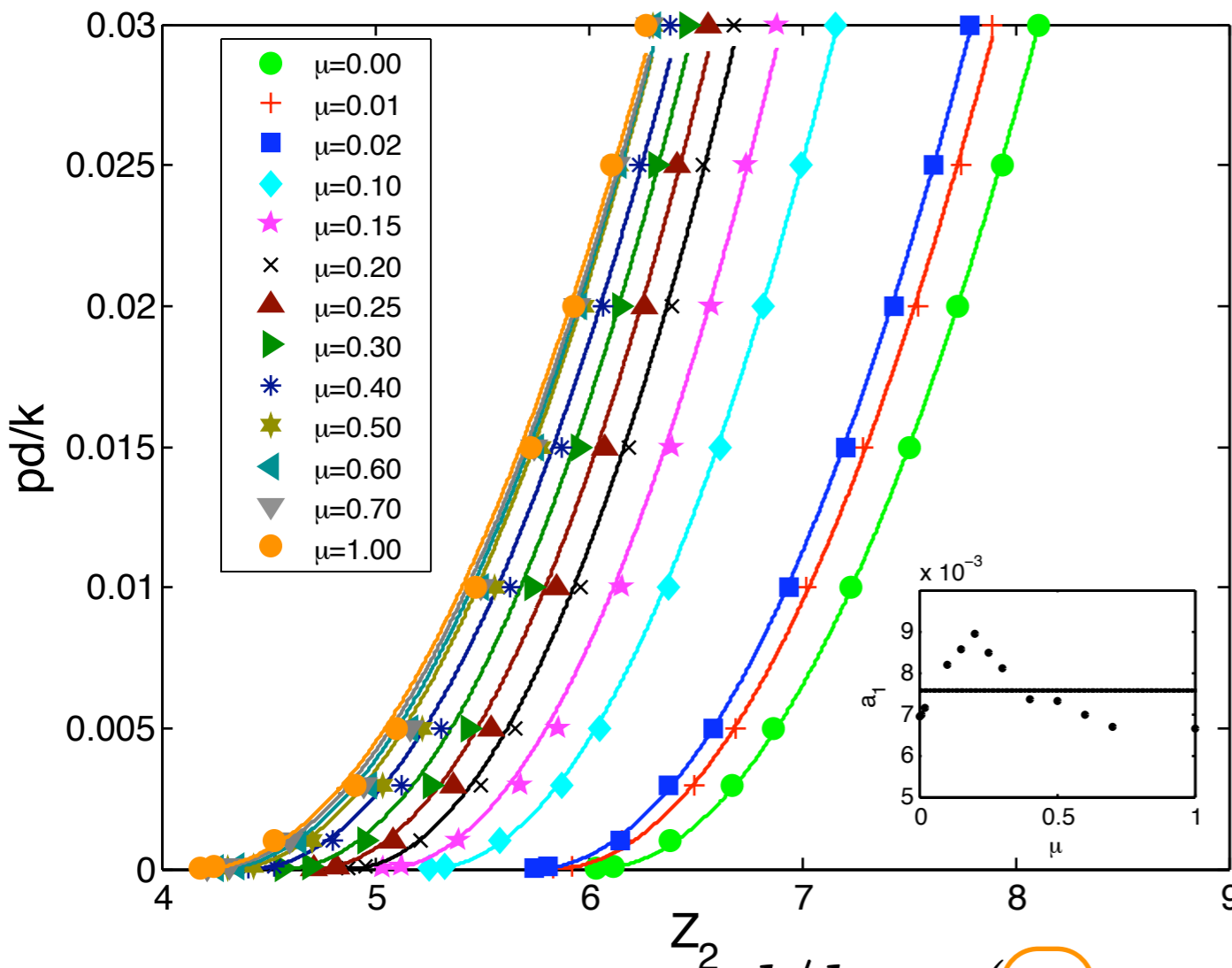
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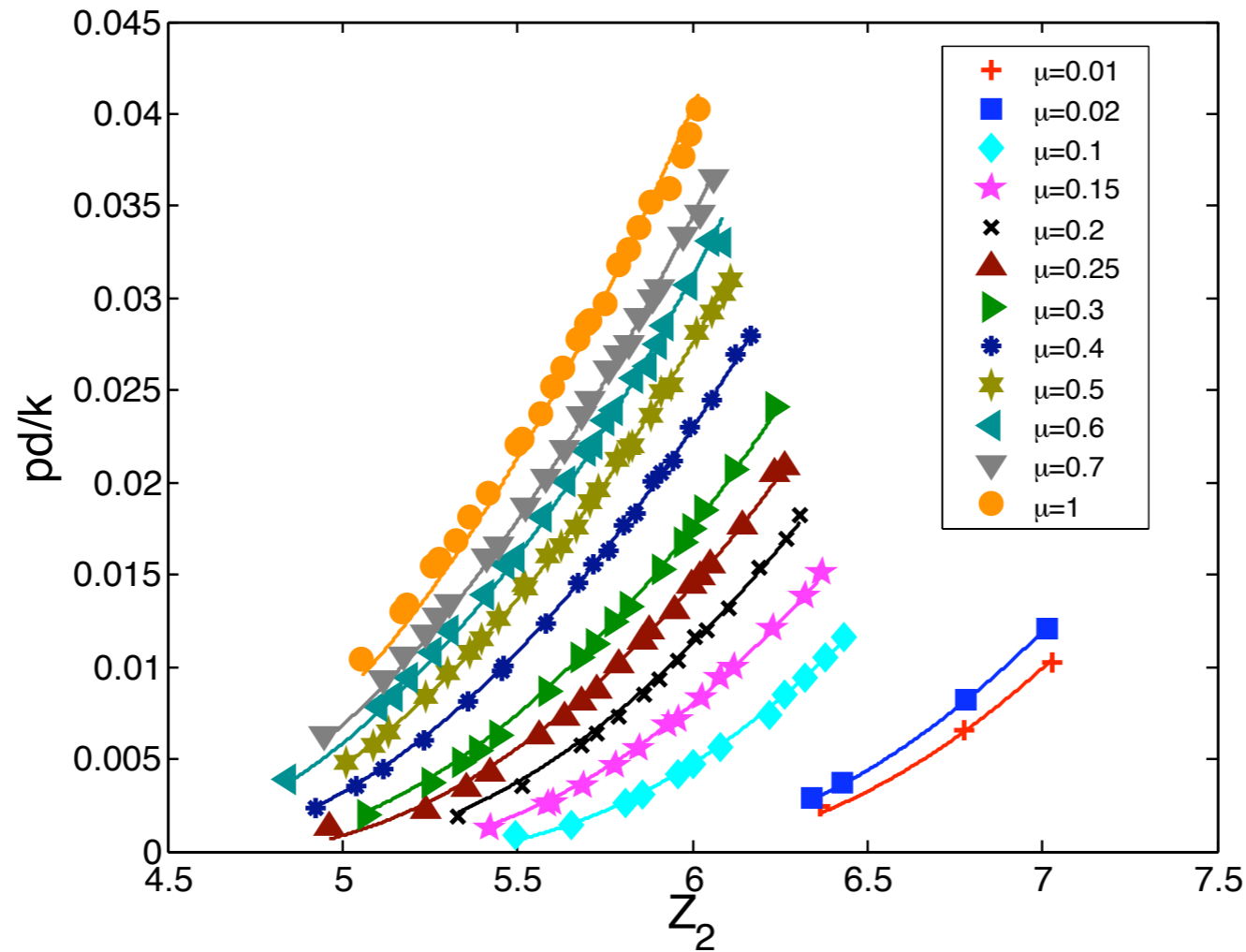
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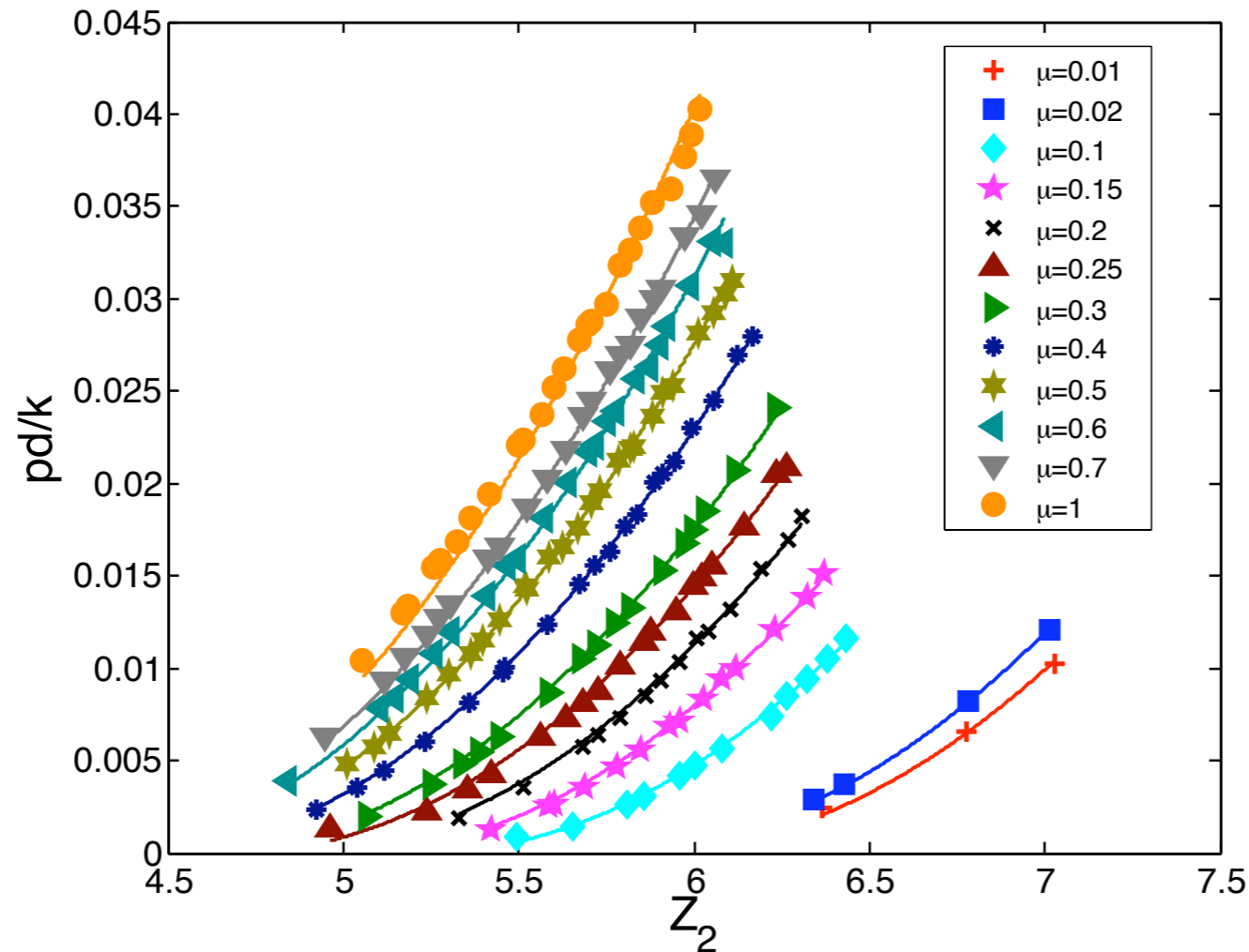
- $a_1$  is a fitting parameter for pressure in isotropic compression
- It fluctuates in a small range and is modeled as a constant.
- Particle friction drives the jamming transition point,  $Z_c$ , to smaller values at higher friction; but scaling is universal.

# Incorporating particle friction: shear pressure



$$pd/k = (a_1 + a_2|A|)(Z - Z_c)^2$$

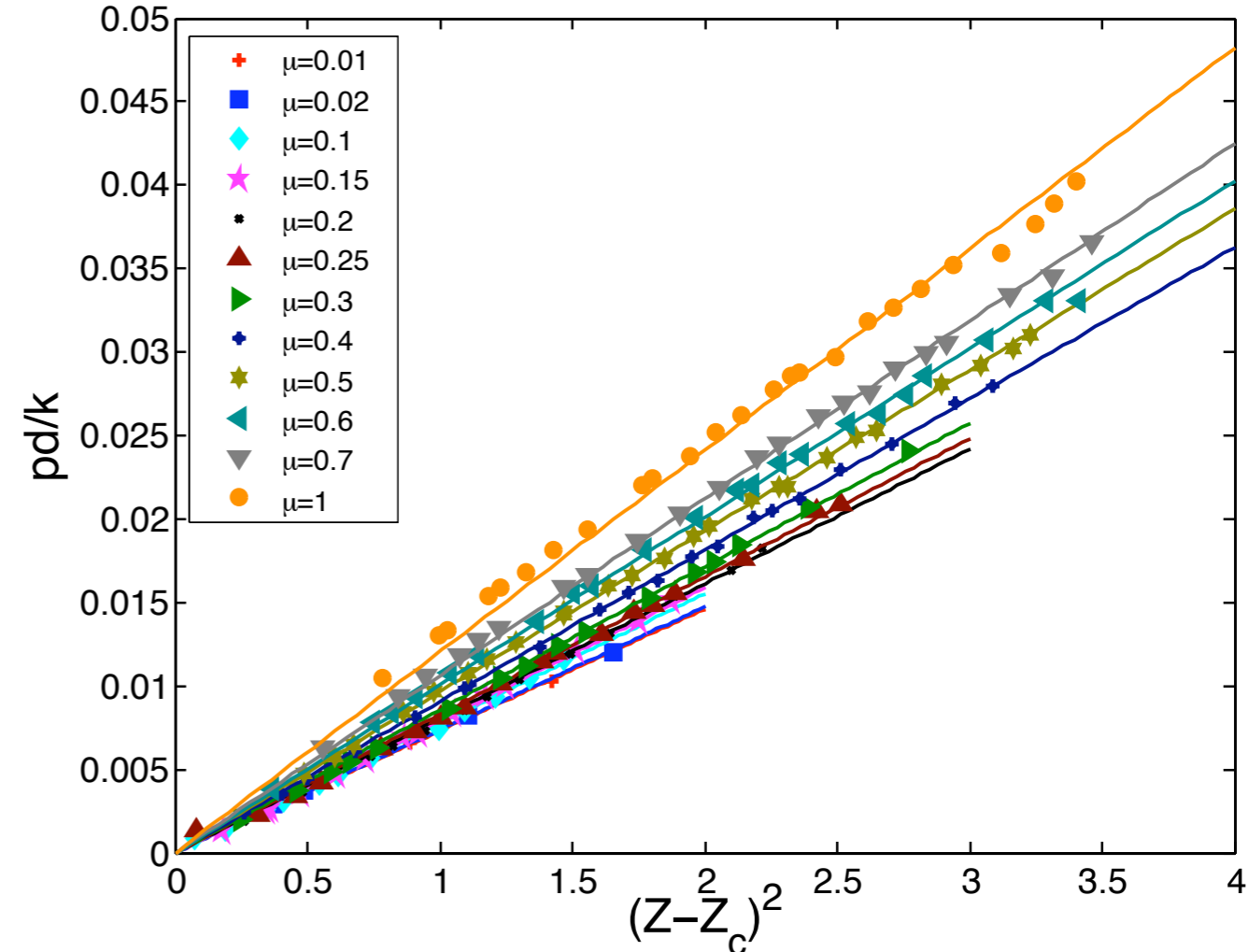
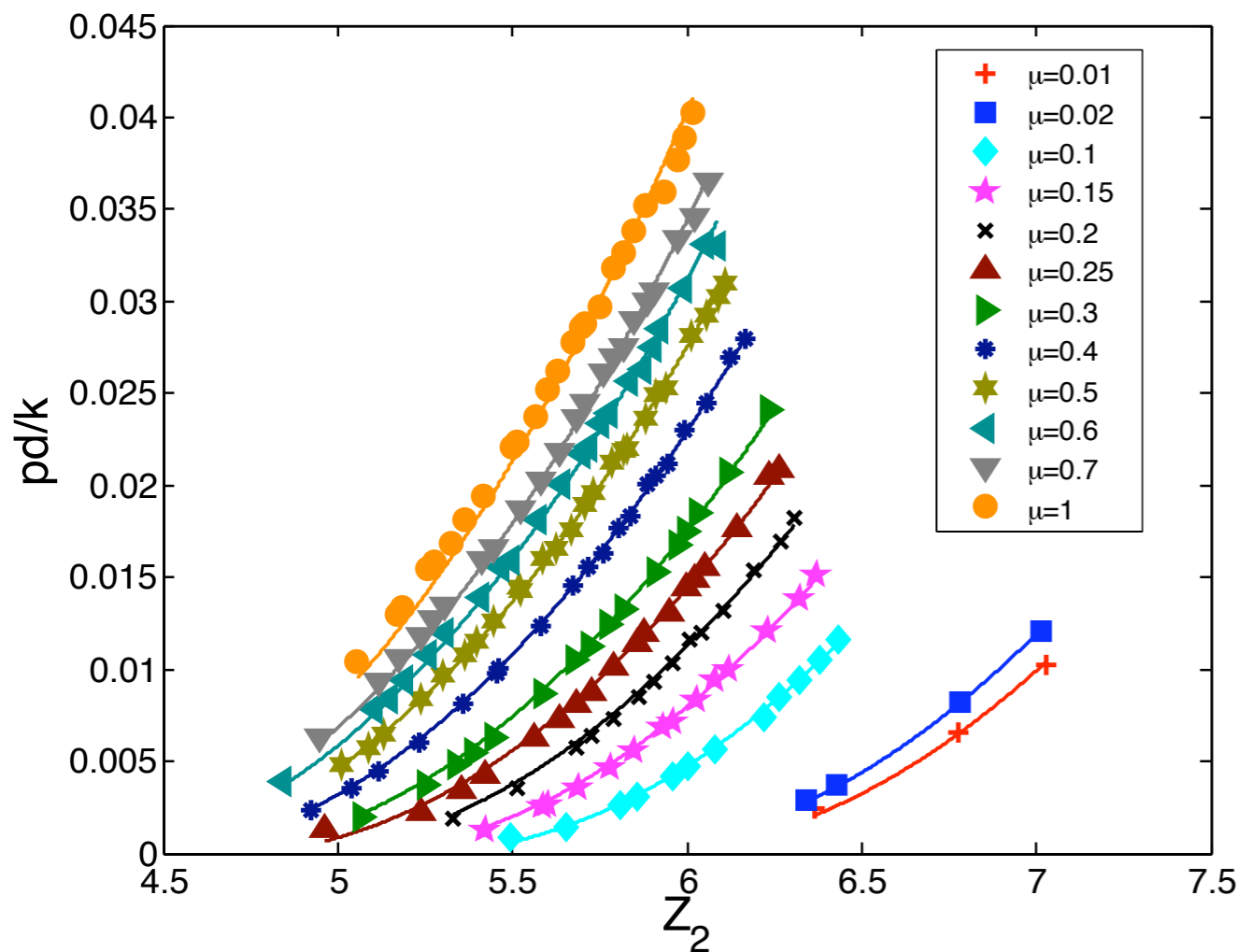
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$$pd/k = (a_1 + a_2|A|)(Z - Z_c)^2$$

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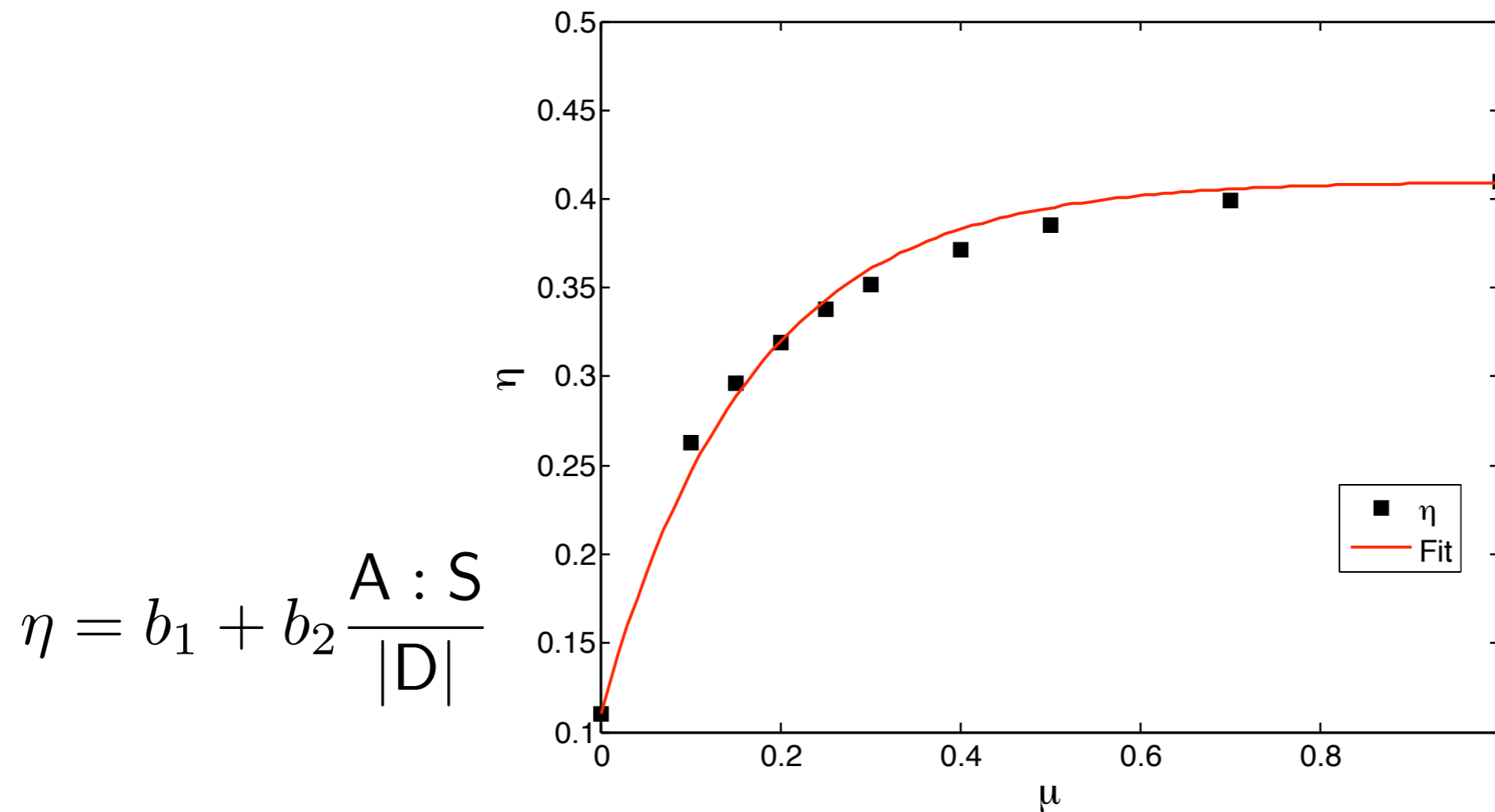
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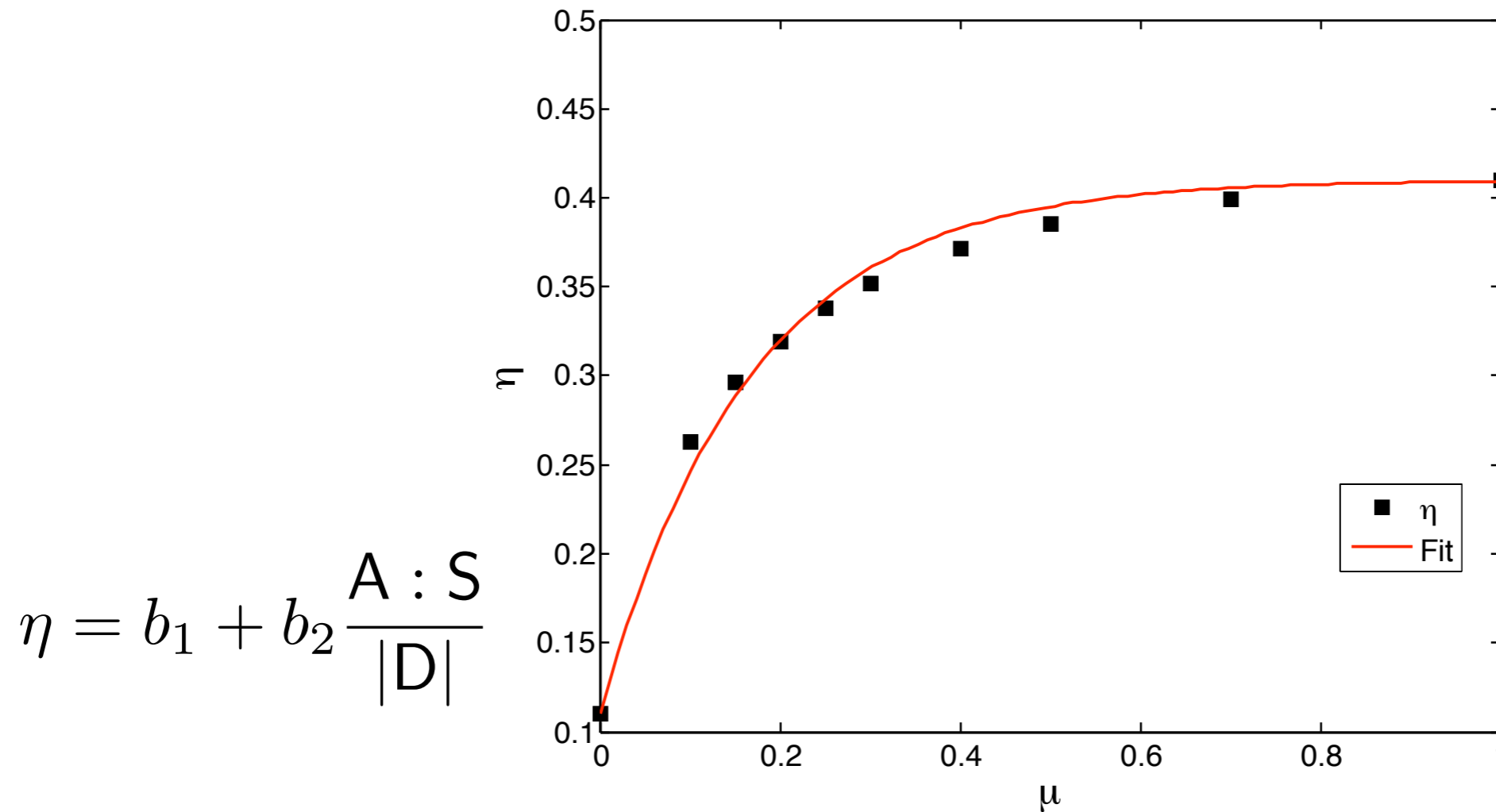
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- $a_2$  is modeled as a linear function of particle friction.

# Incorporating particle friction: shear stress ratio

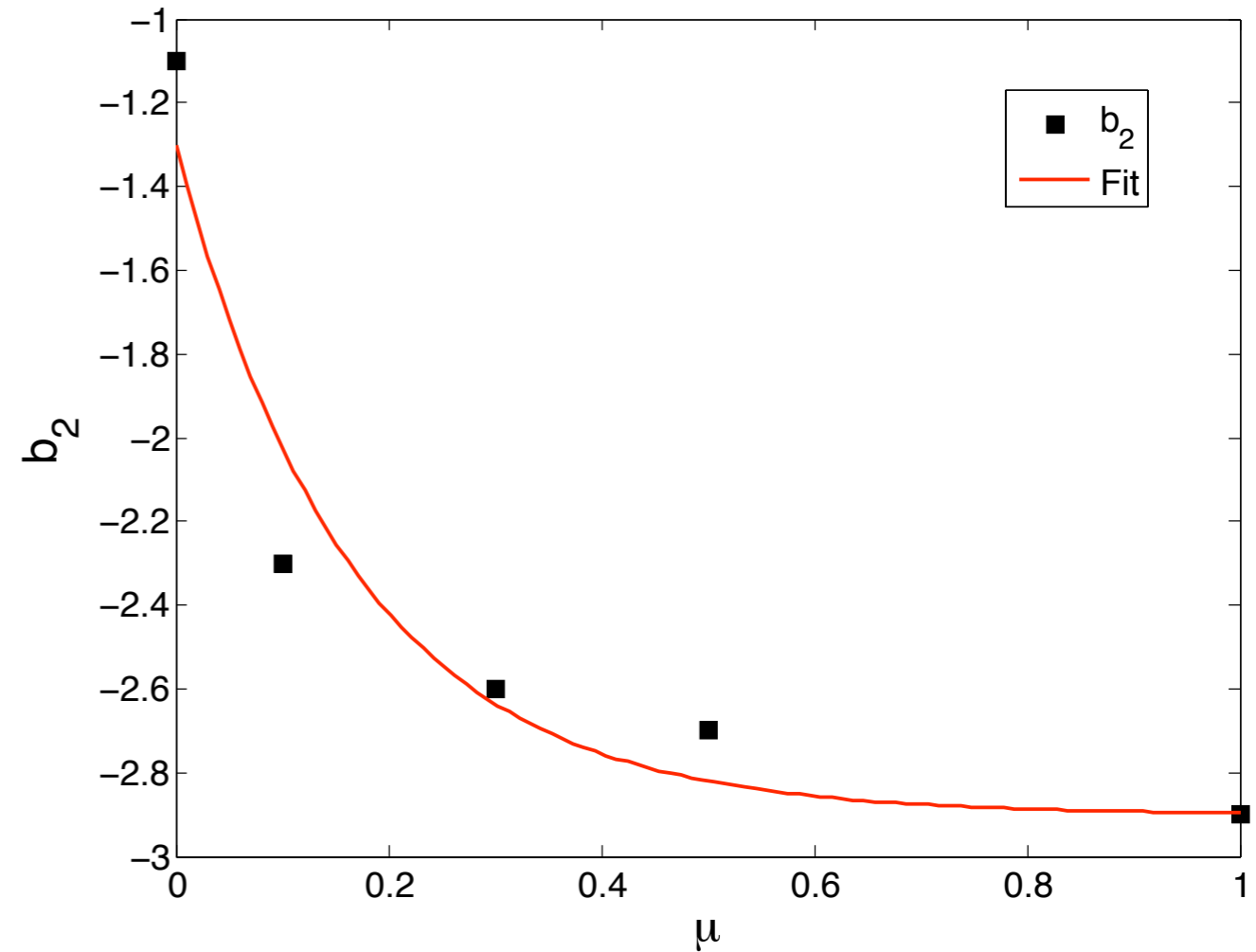
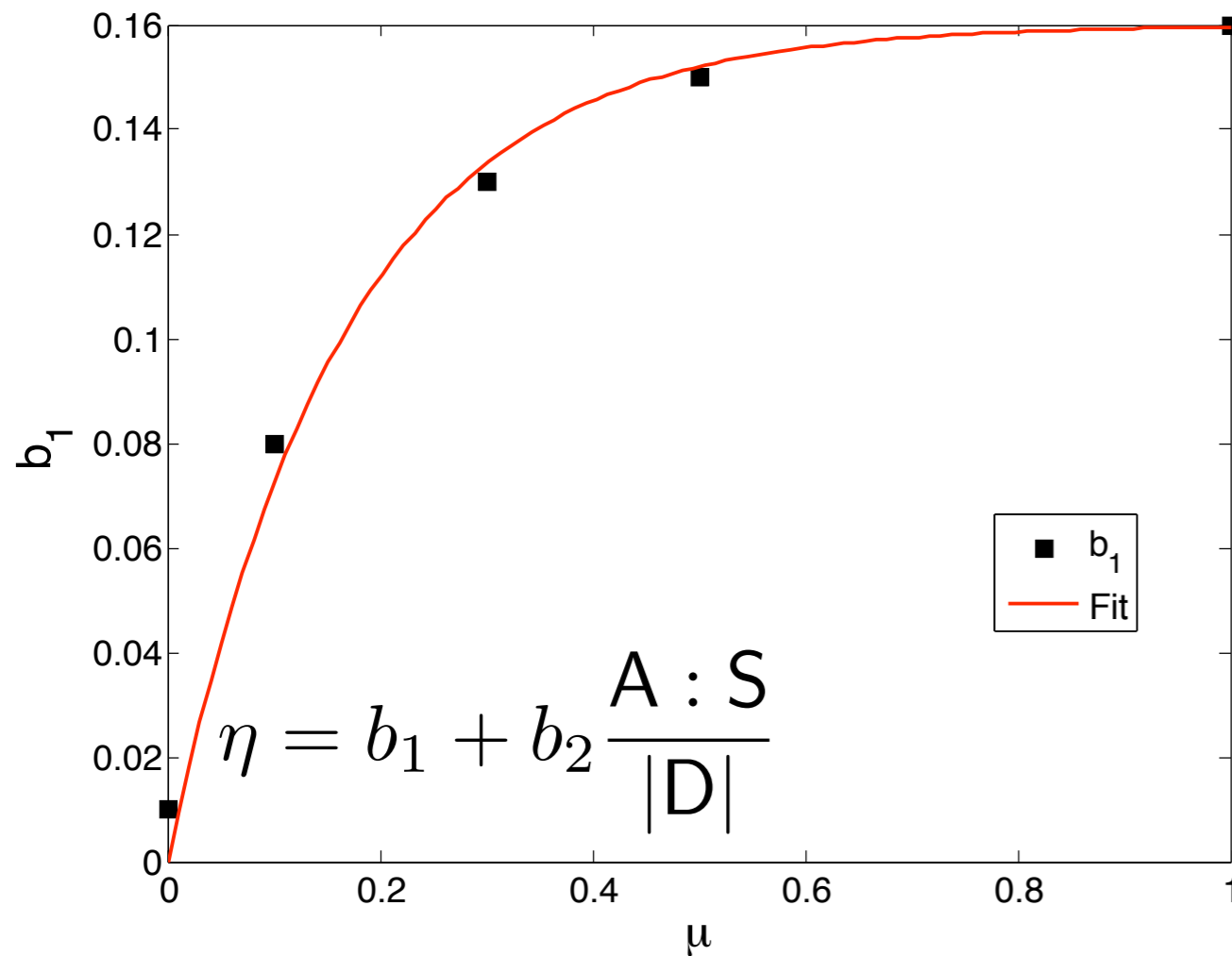


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- $\eta$  is a function of particle friction agreeing with previous studies.\*
- $b_1$  and  $b_2$  vary with particle friction as:
 
$$b_1 = -0.16e^{-6\mu} + 0.16$$

$$b_2 = 1.6e^{-6\mu} - 2.9$$

## Fabric tensor

$$\dot{\mathbf{A}} = c_1 \mathbf{S} + c_2 |\mathbf{D}| \mathbf{A} + c_3 (\mathbf{A} : \mathbf{D}) \mathbf{A}$$

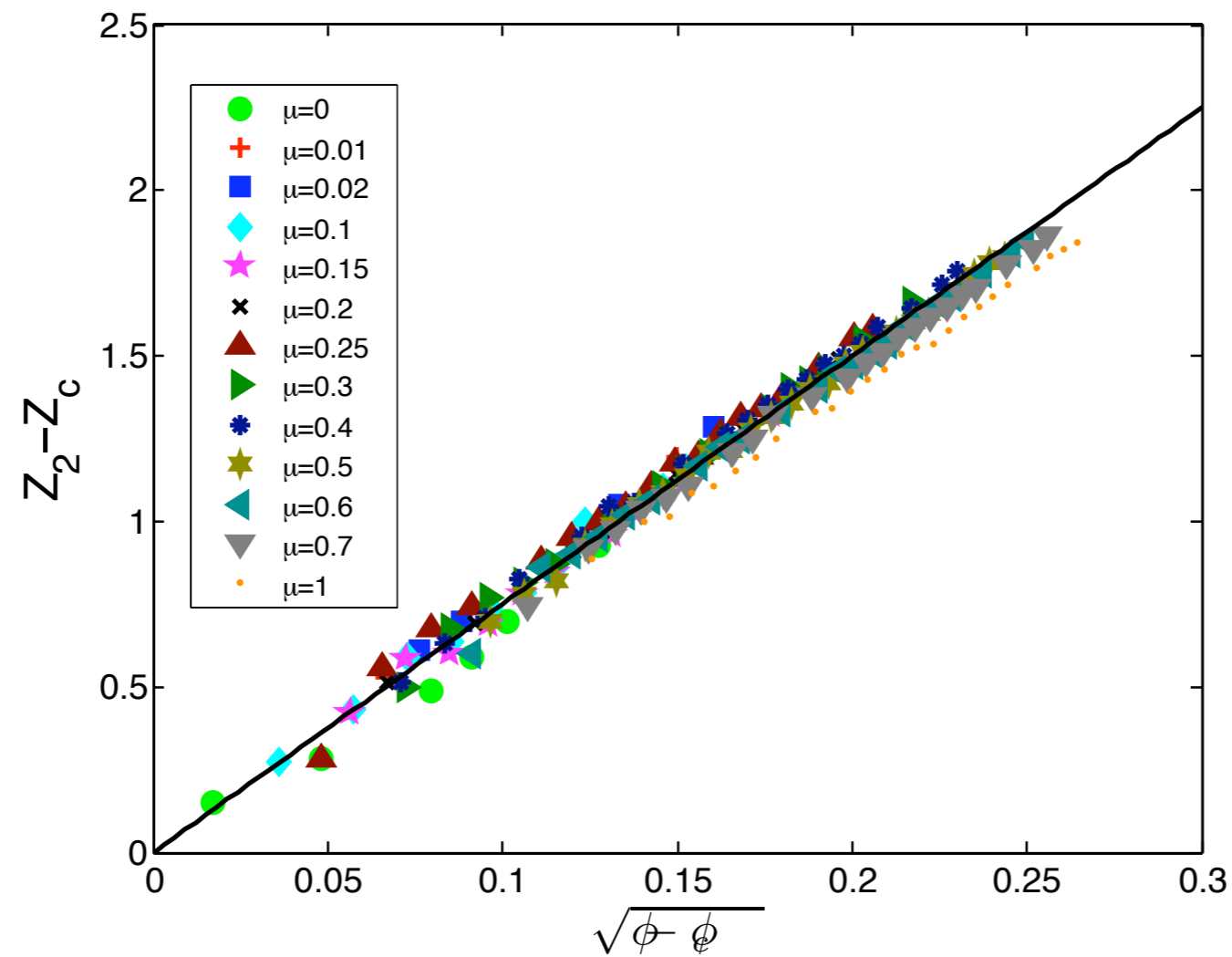
## Coordination number

$$\dot{Z} = d_1 (\mathbf{A} : \mathbf{D} + \chi) + d_2 |\mathbf{D}| (f(\phi) - Z) + d_3 \text{tr}(\mathbf{D})$$

- Material constants  $c_1$ - $c_3$  and  $d_1$ - $d_3$  have little dependence on friction coefficient.
- The main effect on  $Z_c$  and  $\phi_c$  is implemented in the function

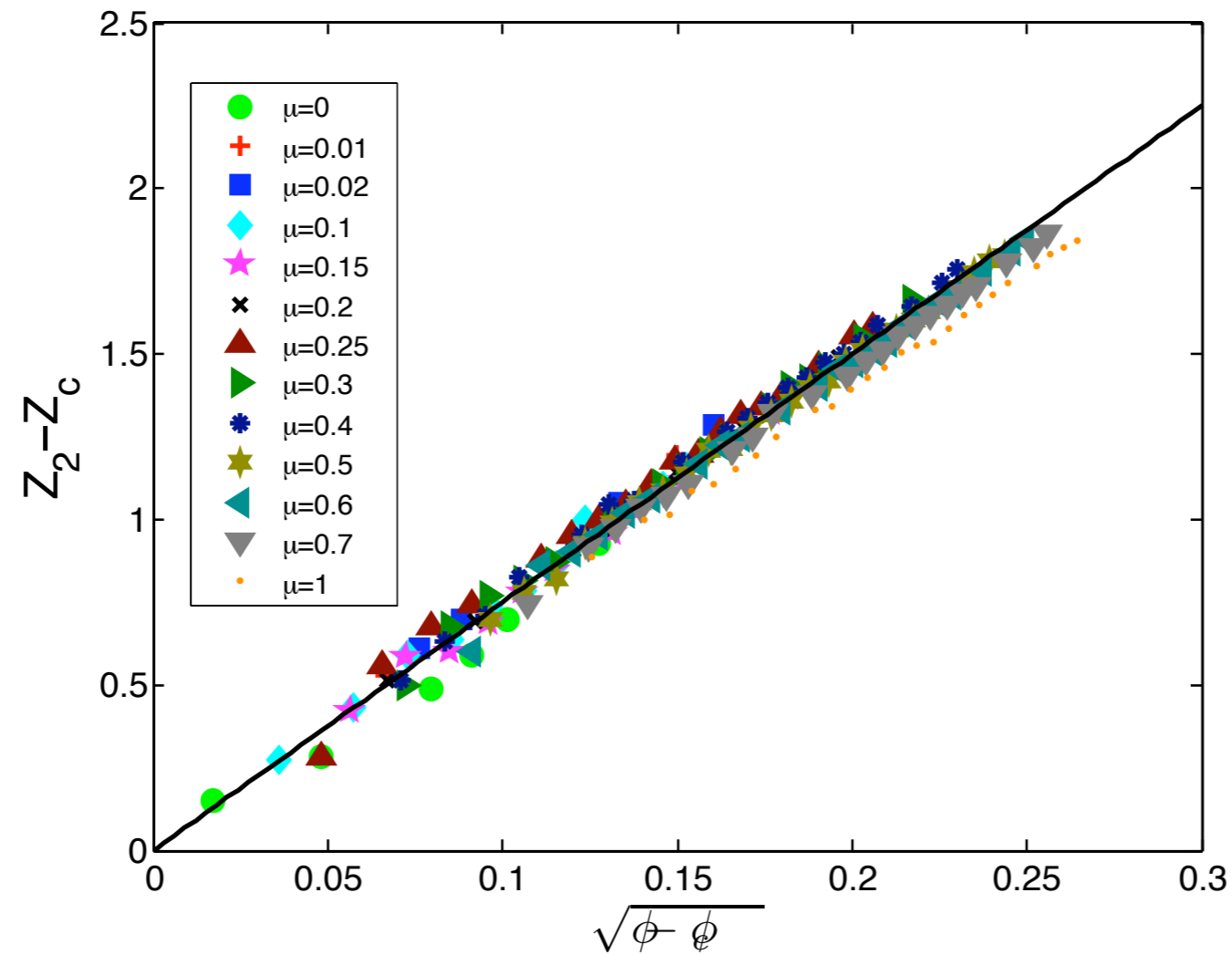
$$f(\phi) = Z_c + \beta_1 (\phi - \phi_c)^{\frac{1}{2}}$$

# $Z$ and $\phi$ correlation



$$Z - Z_c = \beta_1 (\phi - \phi_c)^{\frac{1}{2}}$$

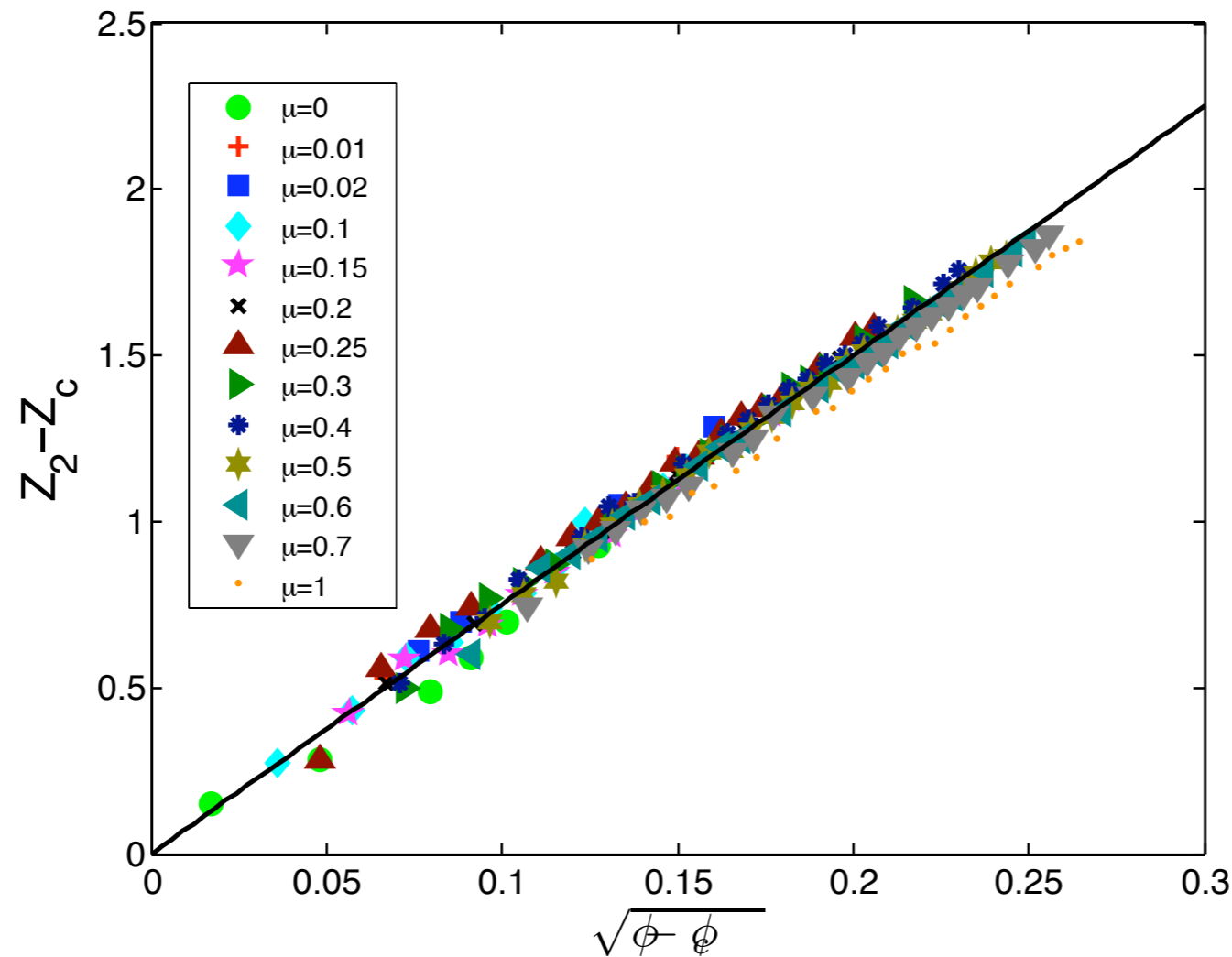
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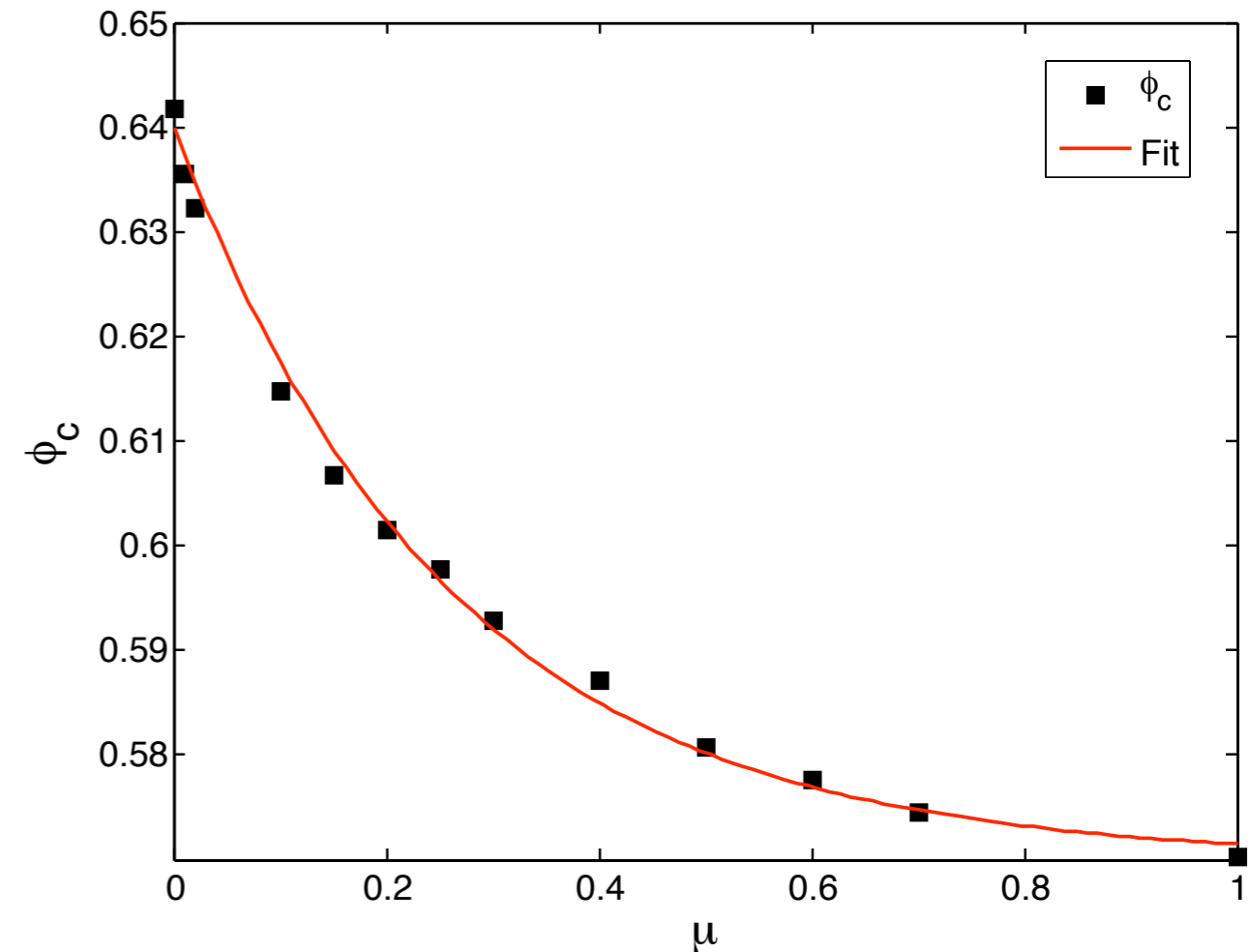
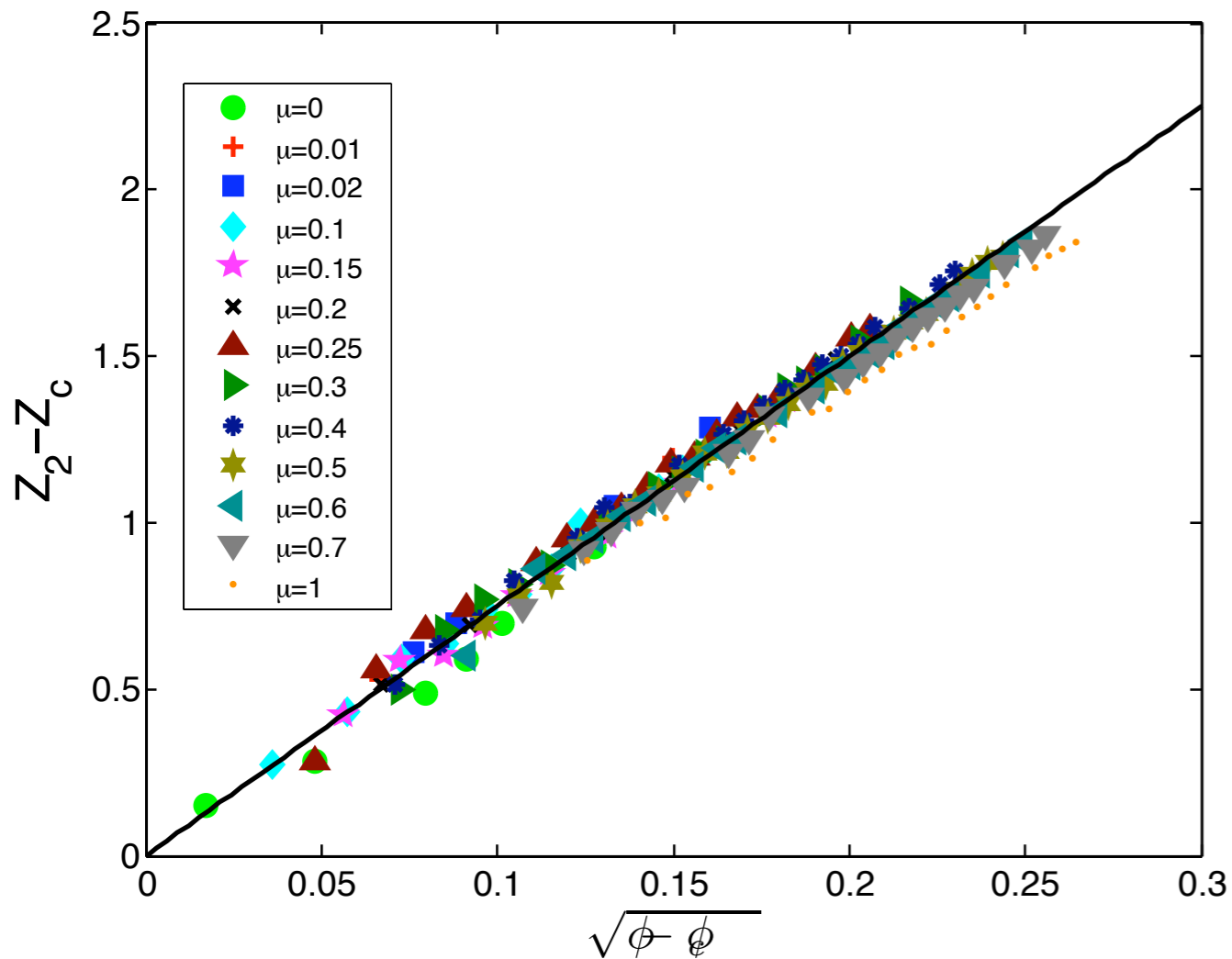
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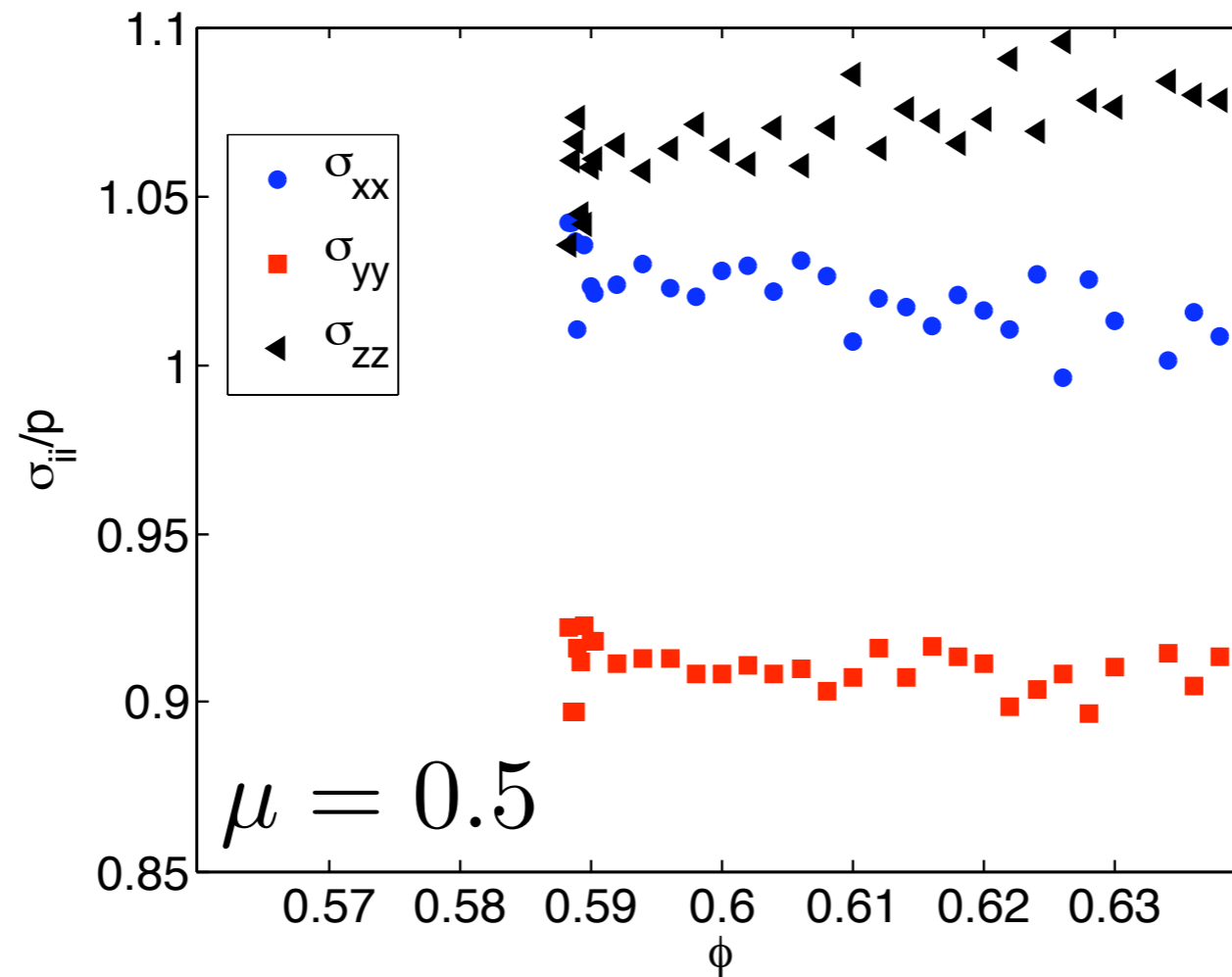
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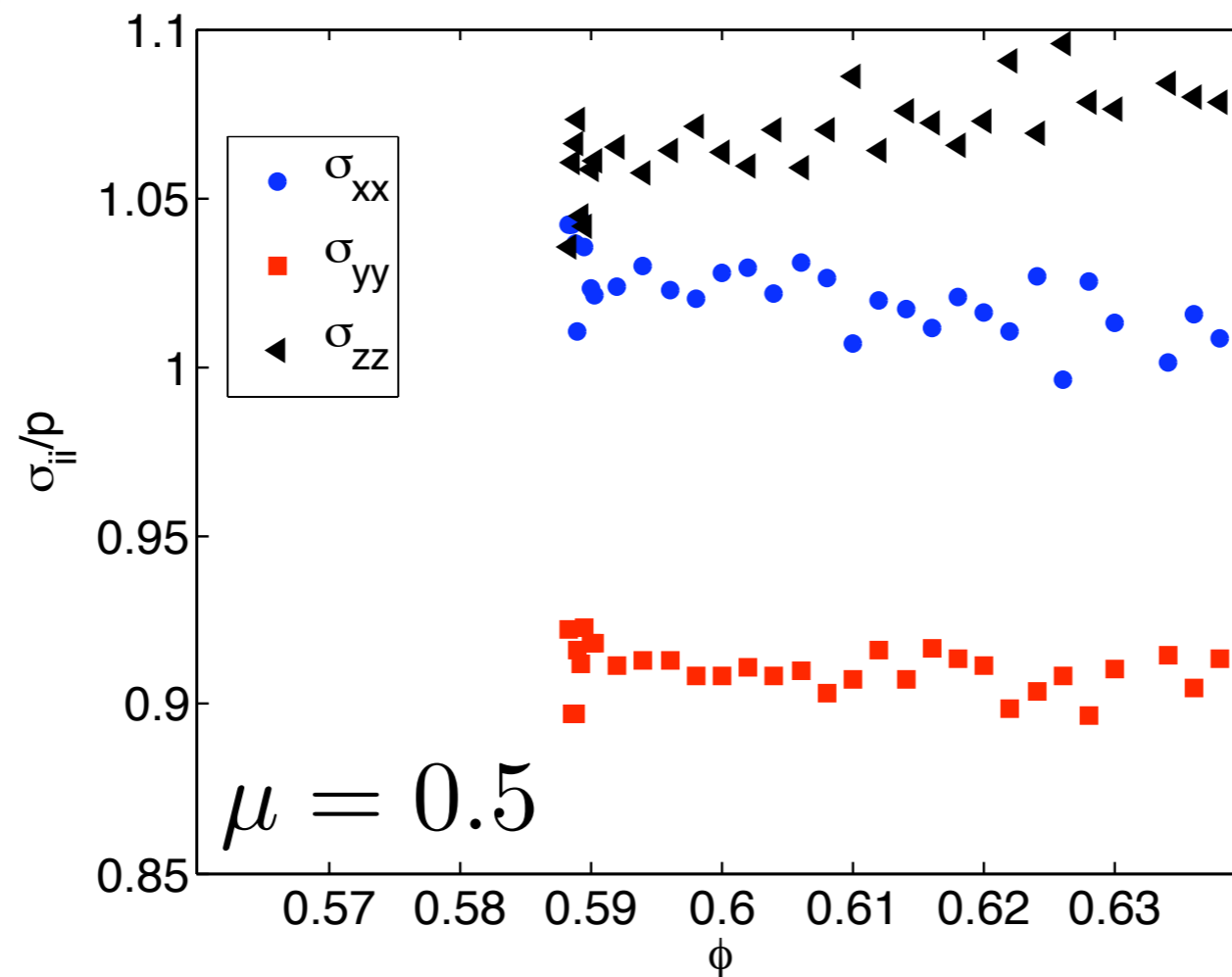
- $\beta_1$  is modeled as a constant.
- $\phi_c$  is determined from this correlation, thus related to jamming transition.
- It decreases with particle friction coefficient.

# Normal stress differences



Steady-state  
simple shear

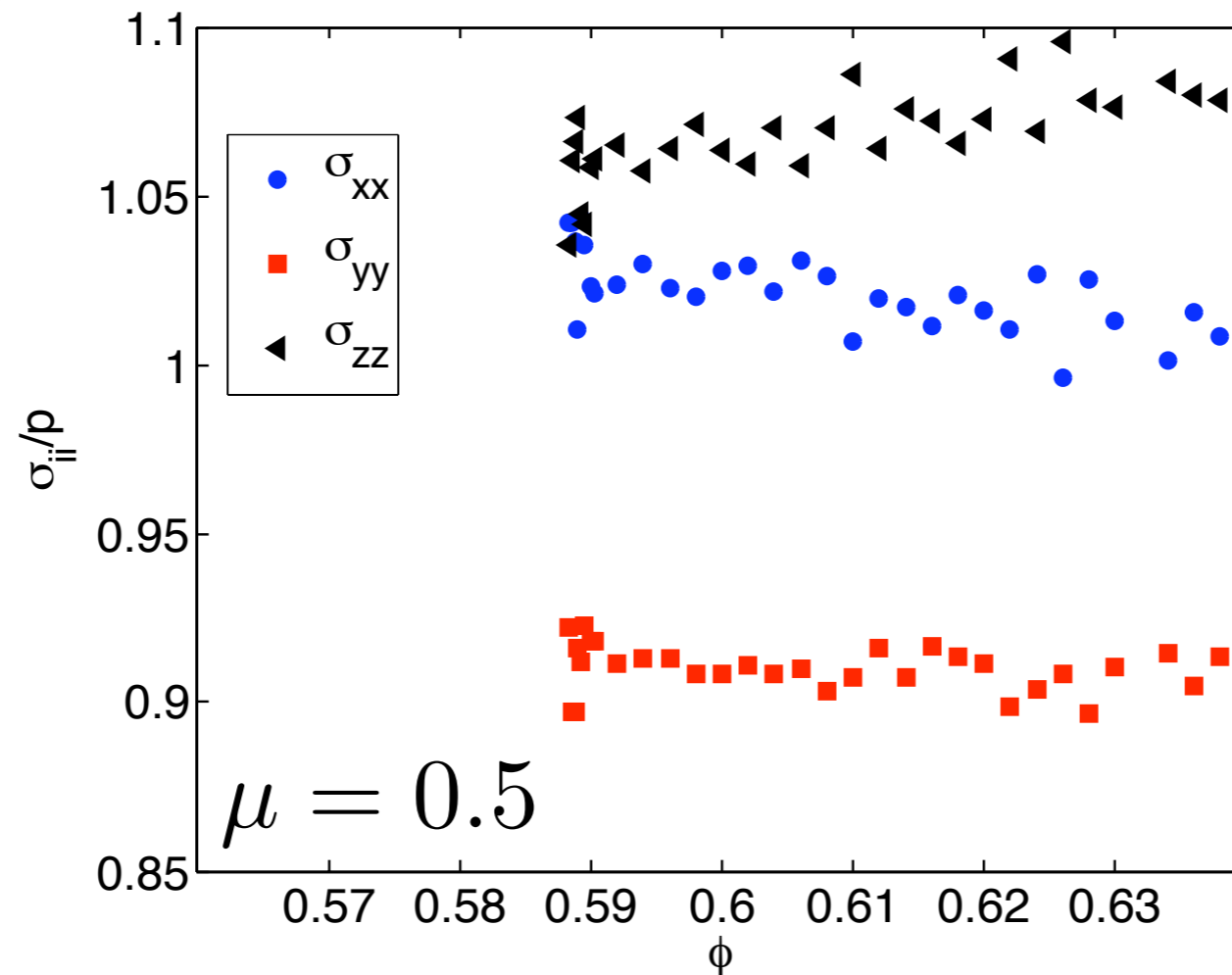
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- Normal stress components are different from each other with deviation of 5-10% from the mean pressure.

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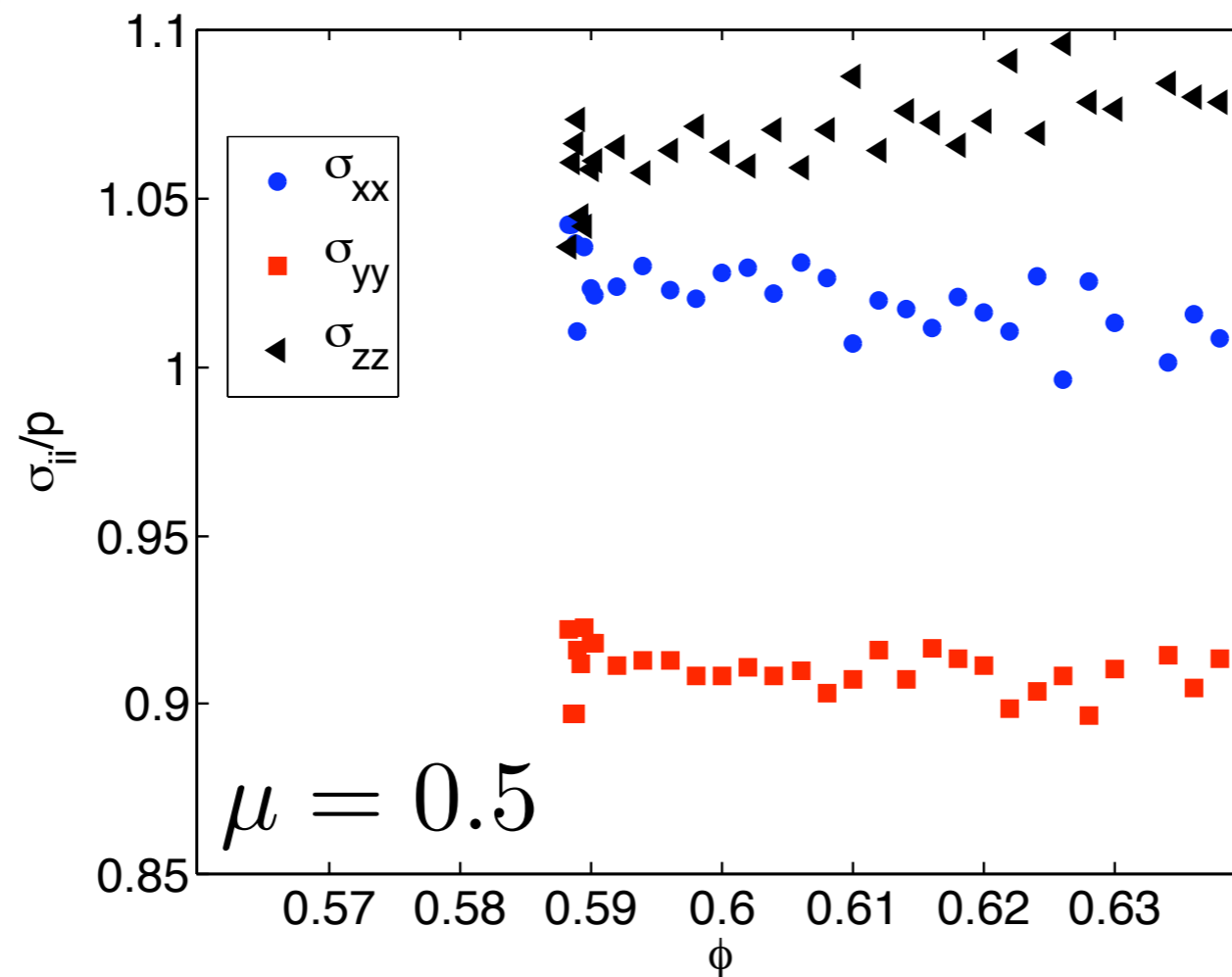


Steady-state  
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- Two extra terms to capture normal stress differences

$$\sigma = pI - p\eta \frac{S}{|D|}$$

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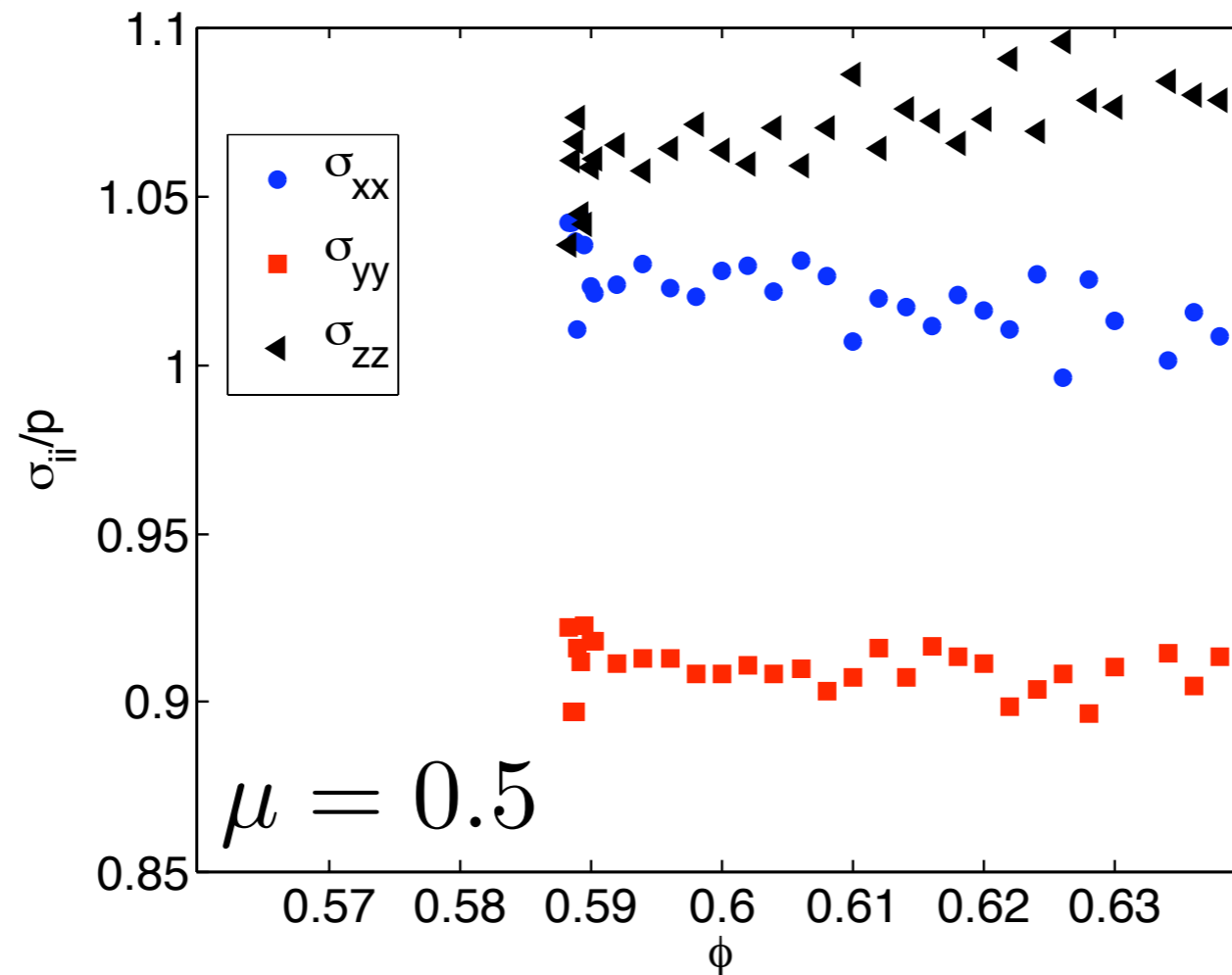


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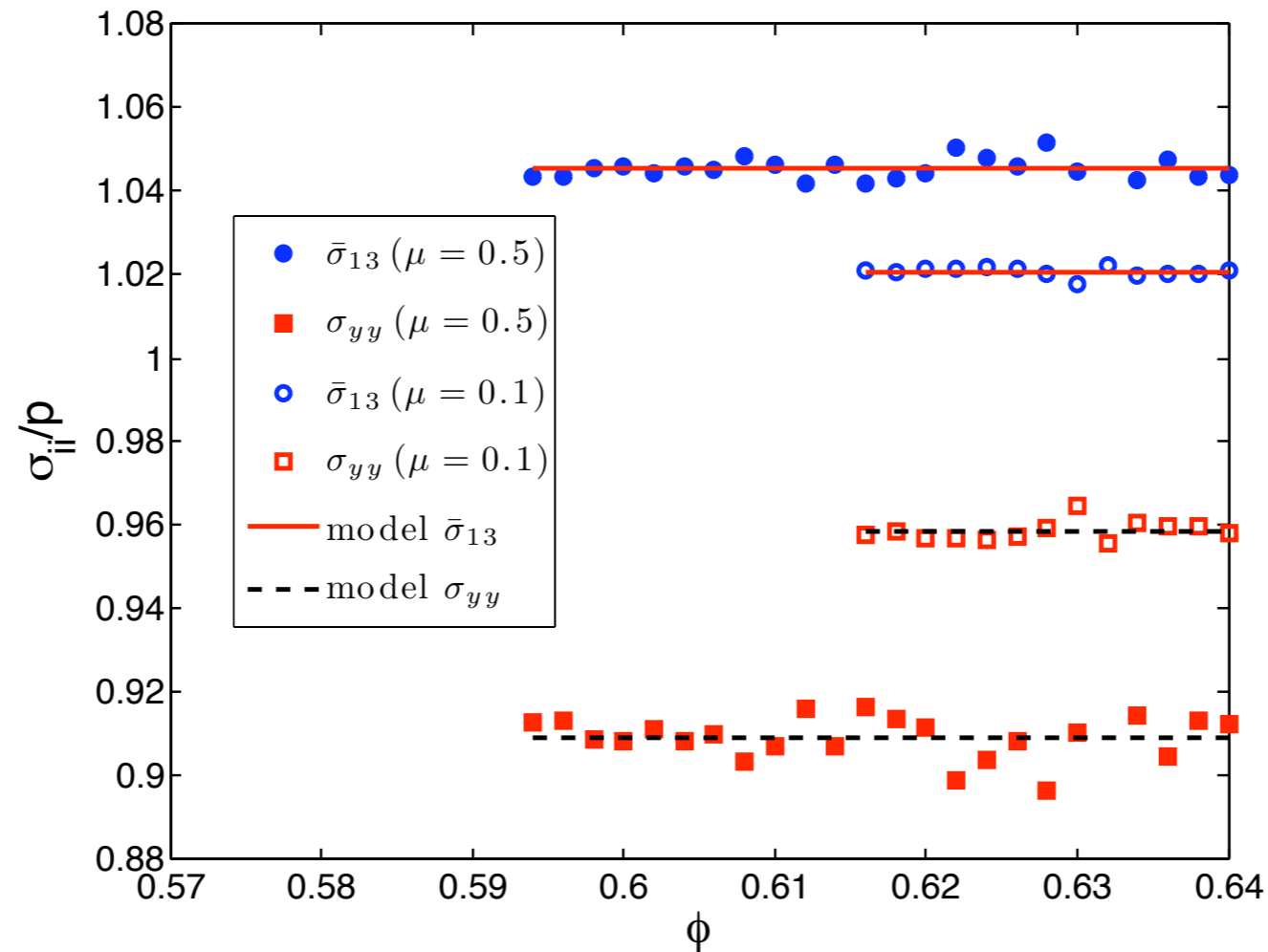


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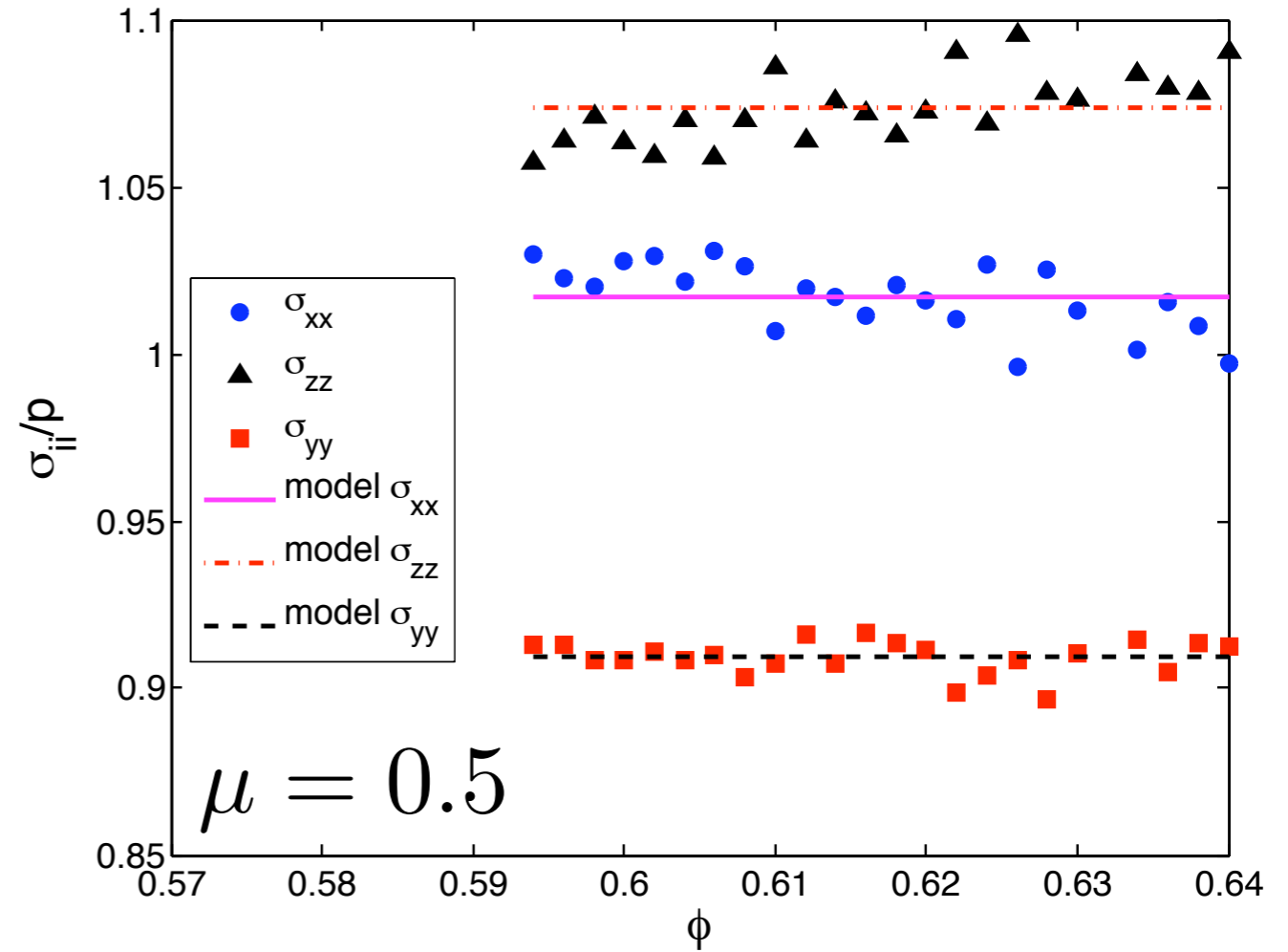
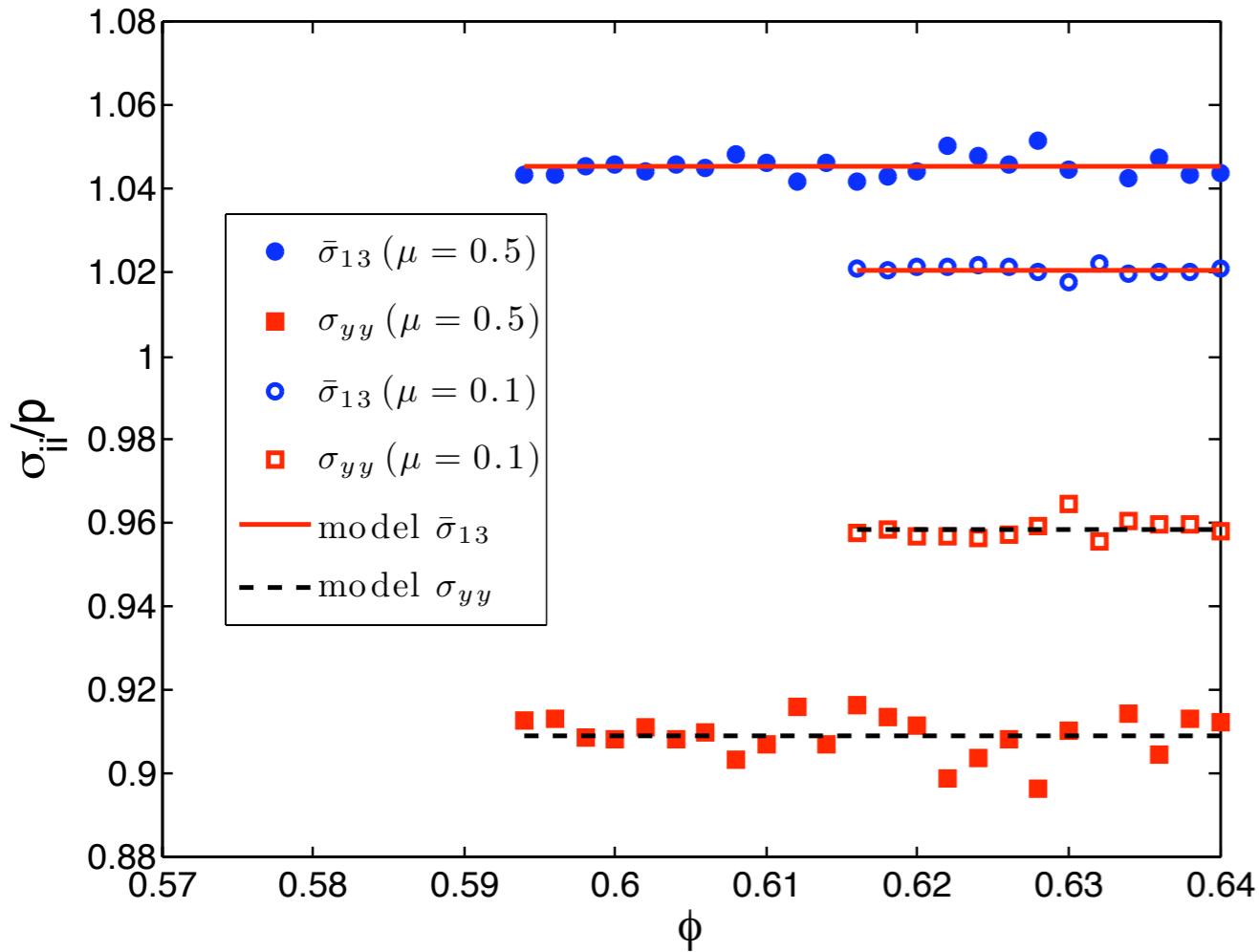
$$\boldsymbol{\sigma} = p\mathbf{I} - p\eta \frac{\mathbf{S}}{|\mathbf{D}|} + a_3 p (\mathbf{A}\hat{\mathbf{D}} + \hat{\mathbf{D}}\mathbf{A} - \frac{2}{3}\mathbf{A} : \hat{\mathbf{D}}\mathbf{I}) + a_4 p \left( \mathbf{A} - \frac{(\mathbf{A} : \mathbf{D})\mathbf{S}}{\mathbf{D} : \mathbf{D}} \right)$$

# Normal stress differences



$$\begin{aligned}\sigma_{xx} &= \sigma_{zz} = p\left(1 + \frac{2}{3}a_3A_{xz}\text{sgn}(\dot{\gamma})\right) \\ \sigma_{yy} &= p\left(1 - \frac{4}{3}a_3A_{xz}\text{sgn}(\dot{\gamma})\right)\end{aligned}$$

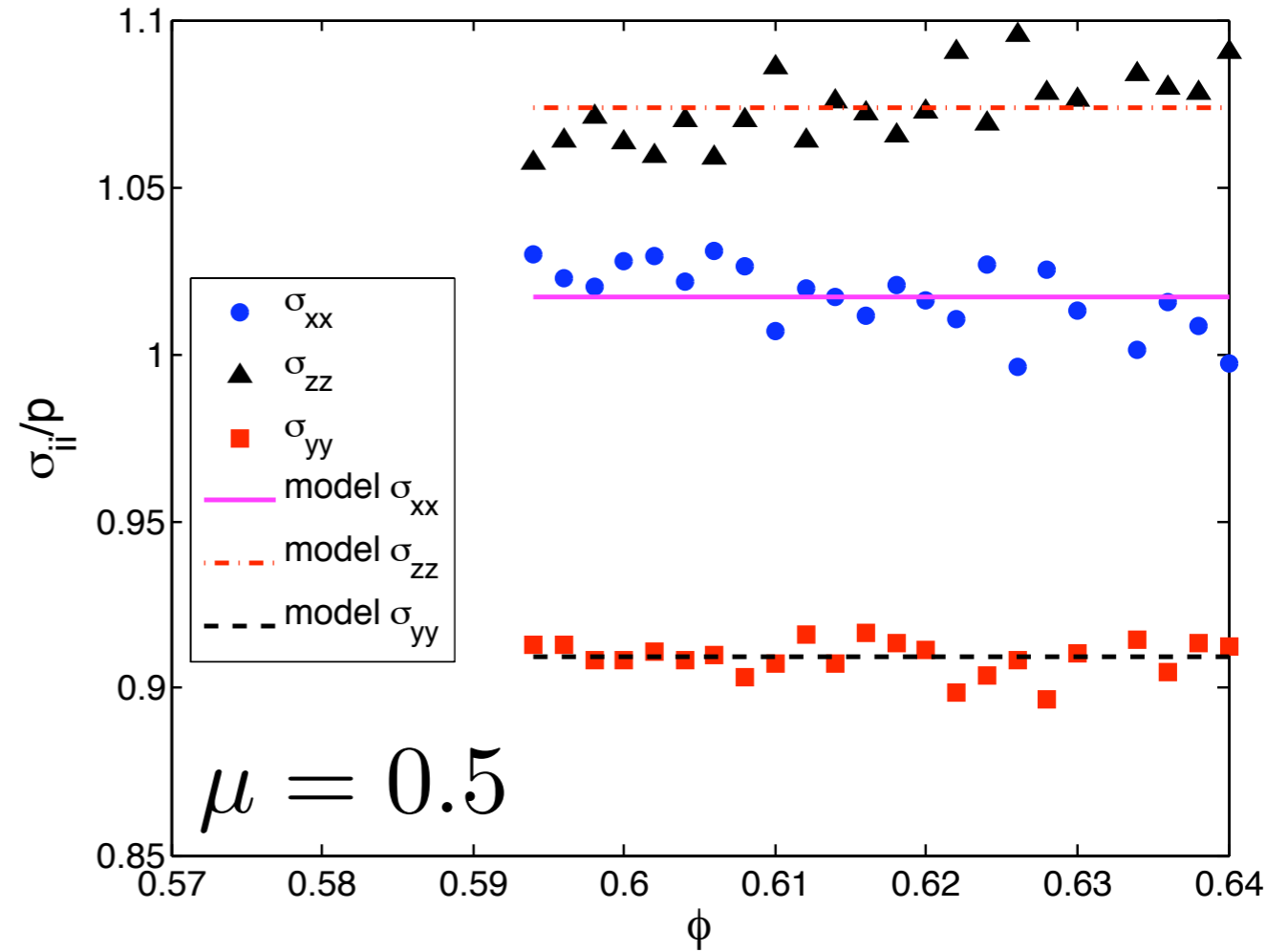
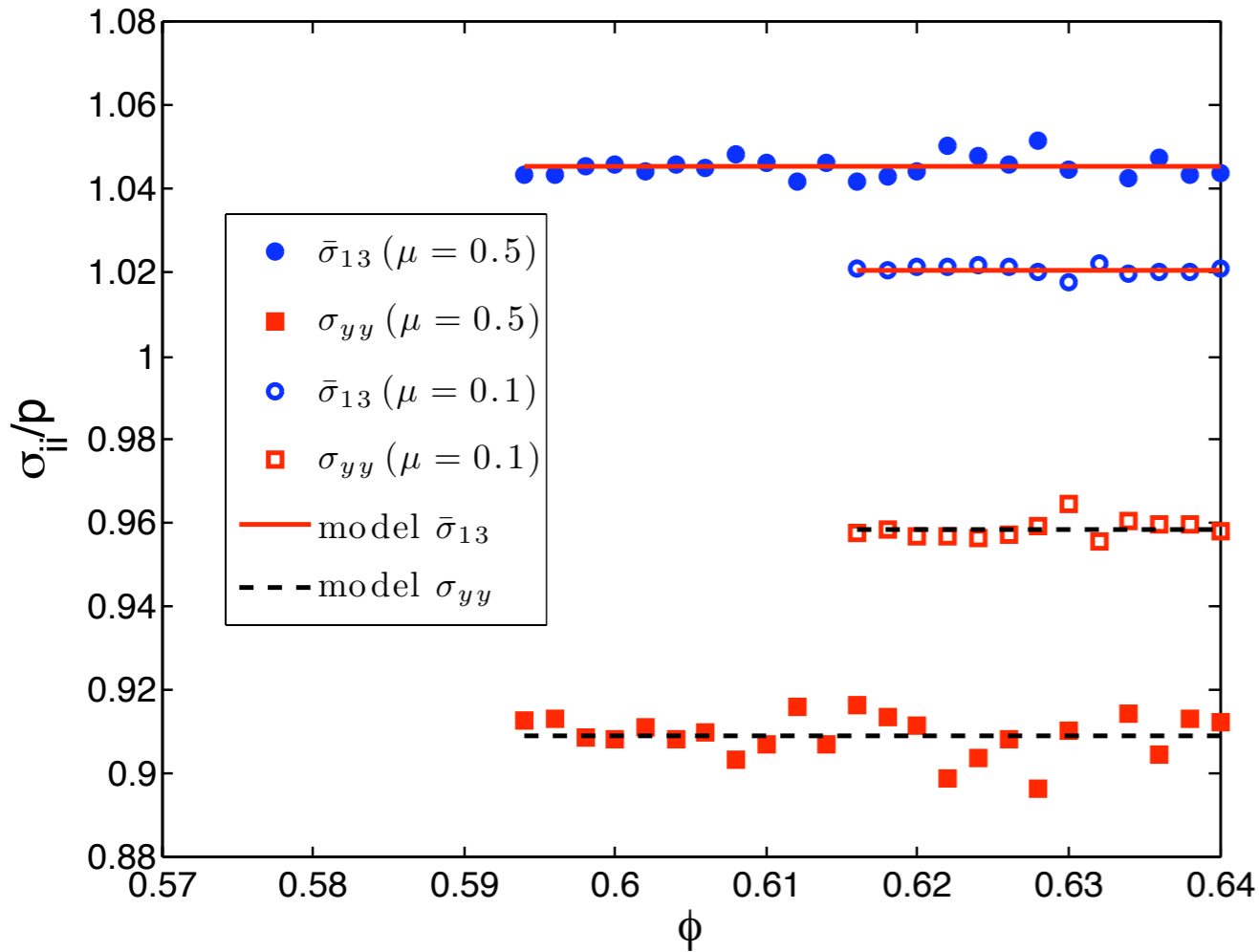
# Normal stress differences



$$\begin{aligned}\sigma_{xx} &= \sigma_{zz} = p\left(1 + \frac{2}{3}a_3A_{xz}\text{sgn}(\dot{\gamma})\right) \\ \sigma_{yy} &= p\left(1 - \frac{4}{3}a_3A_{xz}\text{sgn}(\dot{\gamma})\right)\end{aligned}$$

$$\begin{aligned}\sigma_{xx} &= p\left(1 + \frac{2}{3}a_3A_{xz}\text{sgn}(\dot{\gamma}) + a_4A_{xx}\right) \\ \sigma_{zz} &= p\left(1 + \frac{2}{3}a_3A_{xz}\text{sgn}(\dot{\gamma}) + a_4A_{zz}\right) \\ \sigma_{yy} &= p\left(1 - \frac{4}{3}a_3A_{xz}\text{sgn}(\dot{\gamma})\right)\end{aligned}$$

# Normal stress differences



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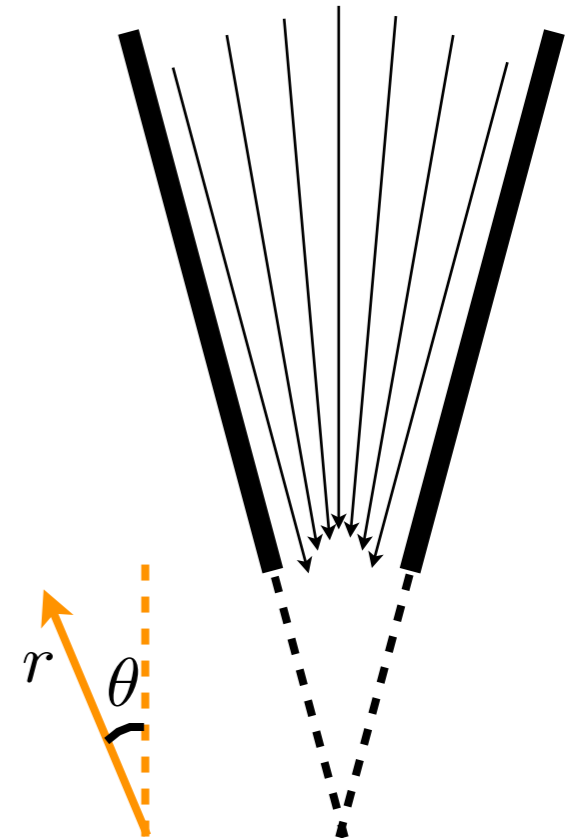
$$\begin{aligned}\sigma_{xx} &= p\left(1 + \frac{2}{3}a_3 A_{xz} \text{sgn}(\dot{\gamma}) + a_4 A_{xx}\right) \\ \sigma_{zz} &= p\left(1 + \frac{2}{3}a_3 A_{xz} \text{sgn}(\dot{\gamma}) + a_4 A_{zz}\right) \\ \sigma_{yy} &= p\left(1 - \frac{4}{3}a_3 A_{xz} \text{sgn}(\dot{\gamma})\right)\end{aligned}$$

$a_3$  and  $a_4$  are also made functions of particle friction

# Application to conical hopper flow



- Classical theories\* do not take account of microstructure change.
- What is the effect of microstructure evolution?
- Compare to the hour-glass theory\*.
- Solve the model for flows in a conical hopper assuming:
  - incompressible flow
  - smooth side walls
  - stress-free surface
  - radial gravity



\* R. M. Nedderman. Statics and Kinematics of Granular Materials.

# One-dimensional equations



- Scaled microstructure and stress equations in a spherical coordinate system

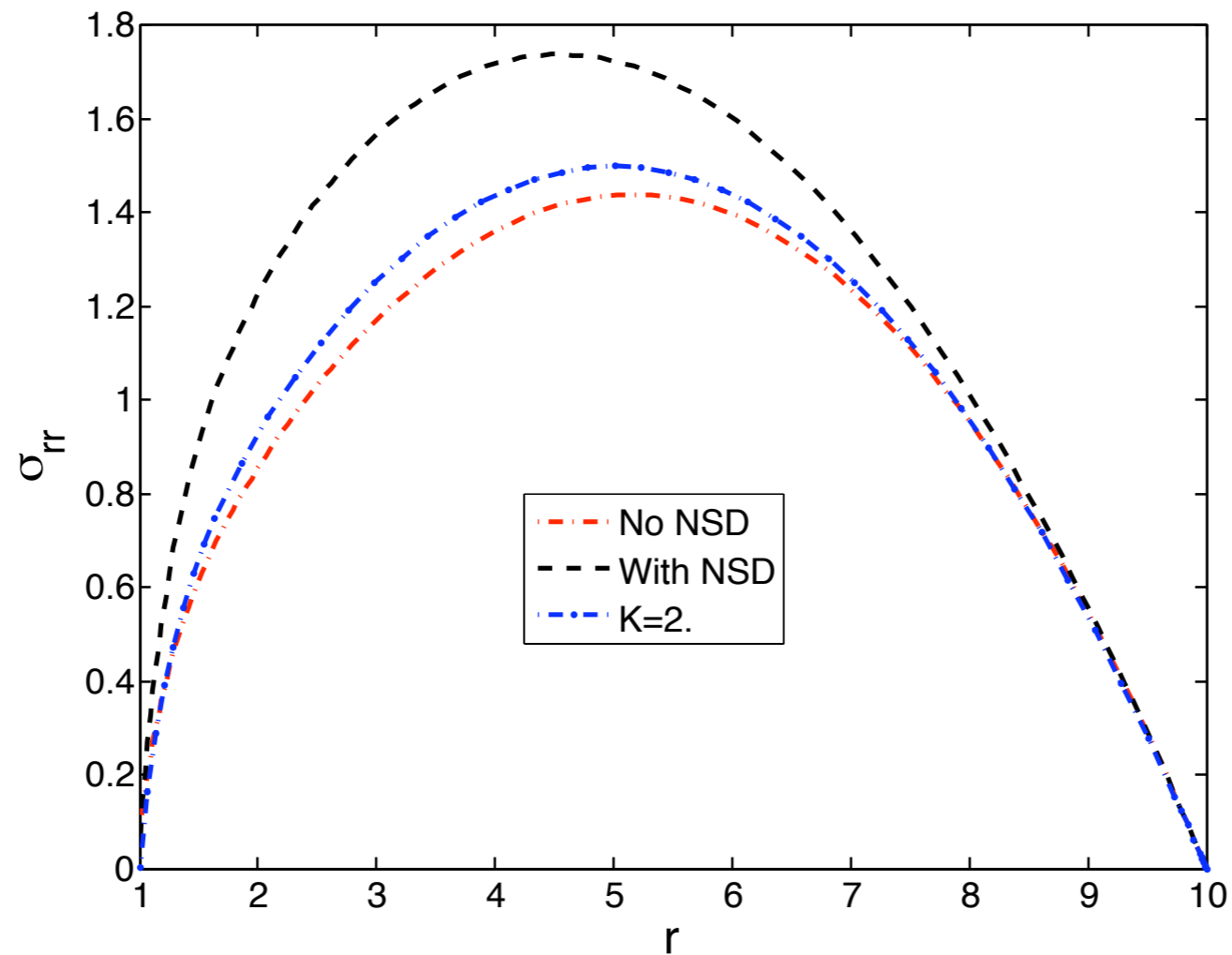
Scaled fabric  $\frac{dA_{rr}}{d\hat{r}} = -\frac{1}{\hat{r}}(2c_1 + \sqrt{3}c_2 A_{rr} + 3c_3 A_{rr}^2)$

Scaled stress  $\frac{d\hat{\sigma}}{d\hat{r}} = \frac{2\phi\hat{V}^2}{\hat{r}^5} + \frac{2(\kappa - 1)\hat{\sigma}}{\hat{r}} - \phi$

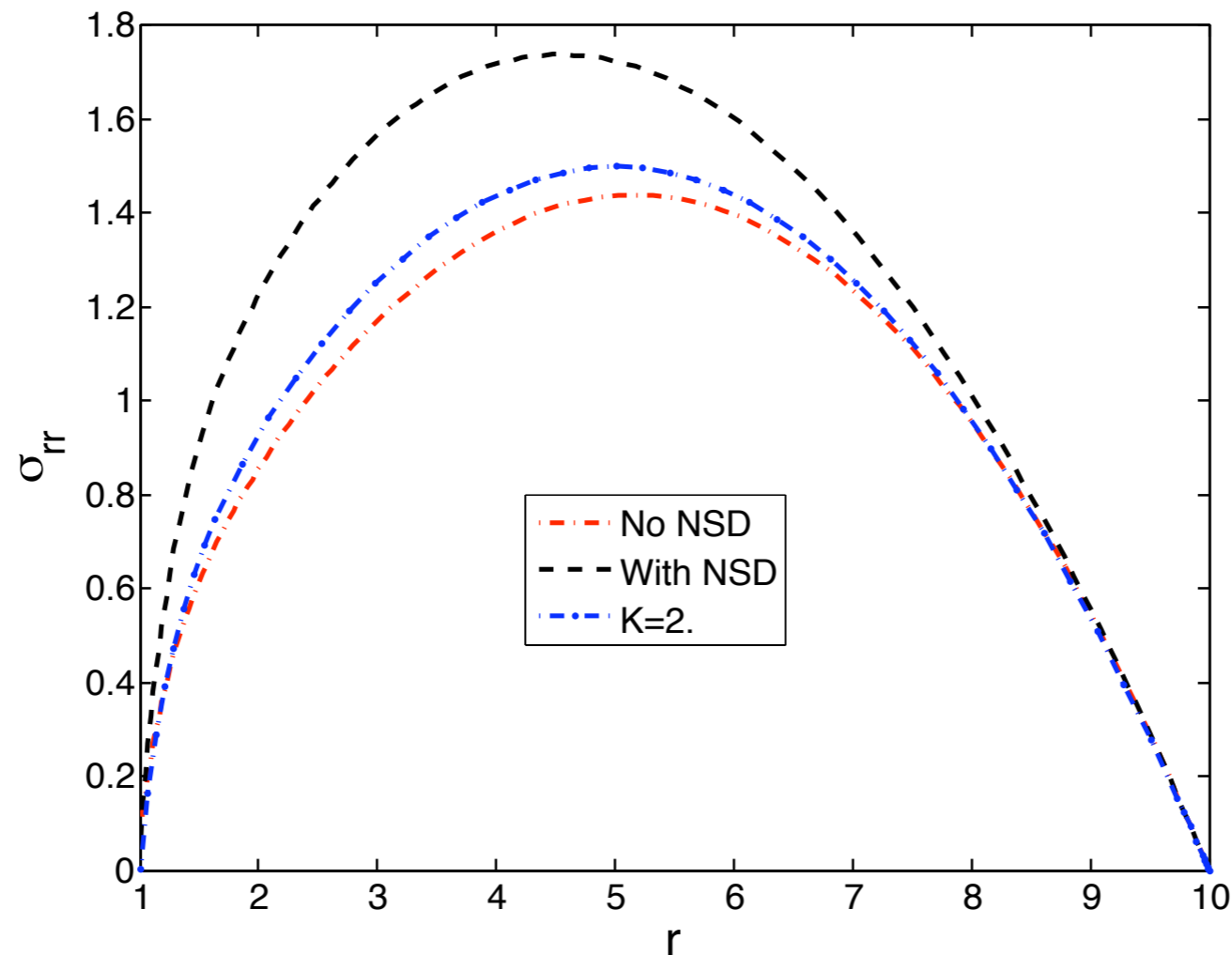
$$\hat{r} = \frac{r}{R_{\text{out}}} \quad \hat{\sigma} = \frac{\sigma}{\rho_s g R_{\text{out}}} \quad \text{Flow rate } \hat{V} = \frac{V}{\sqrt{R_{\text{out}}^5 g}}$$

- $\kappa$  is a function of  $\eta$  in our model, but is constant in the hour-glass theory.

# Predictions of stress and macroscopic friction

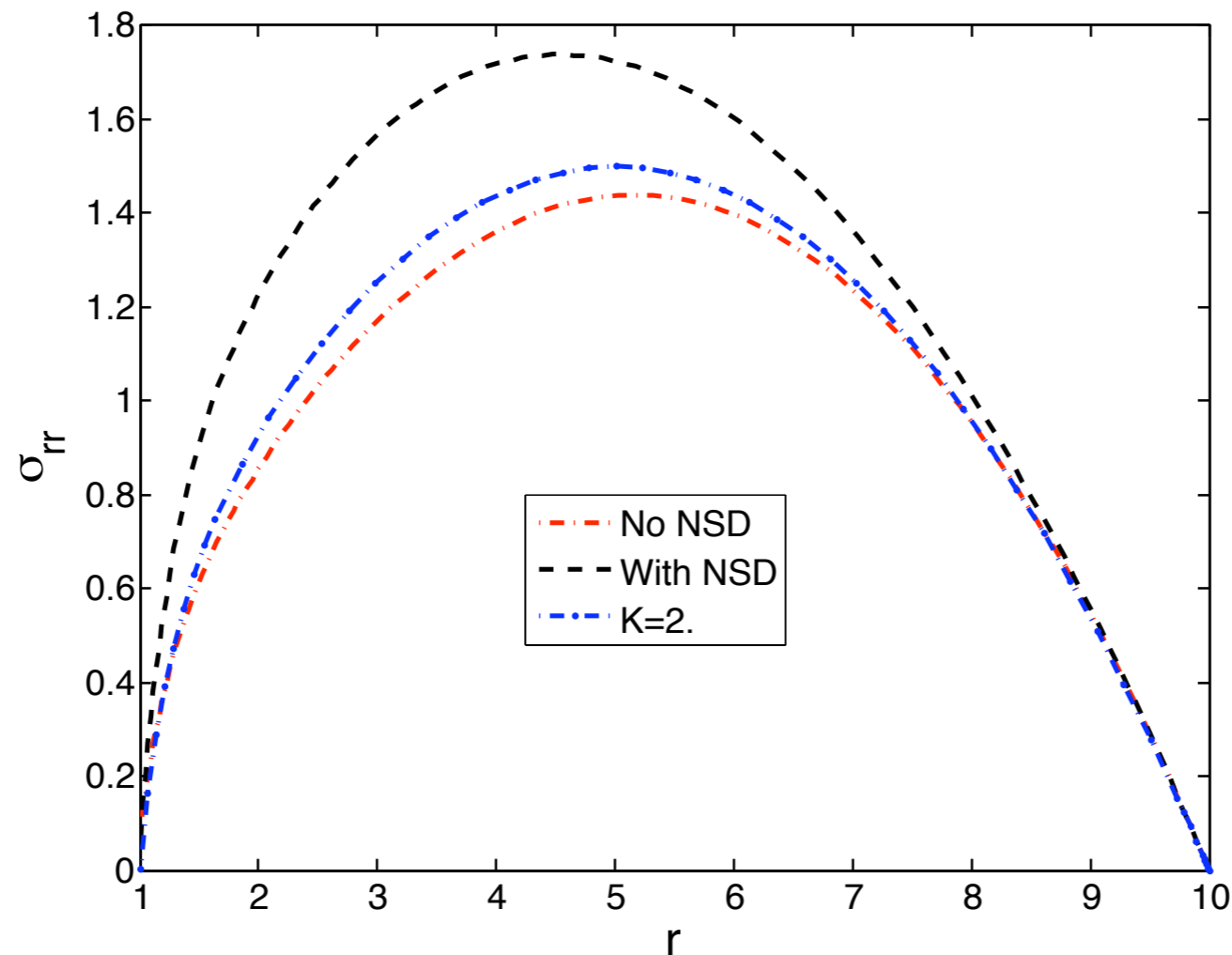


# Predictions of stress and macroscopic friction



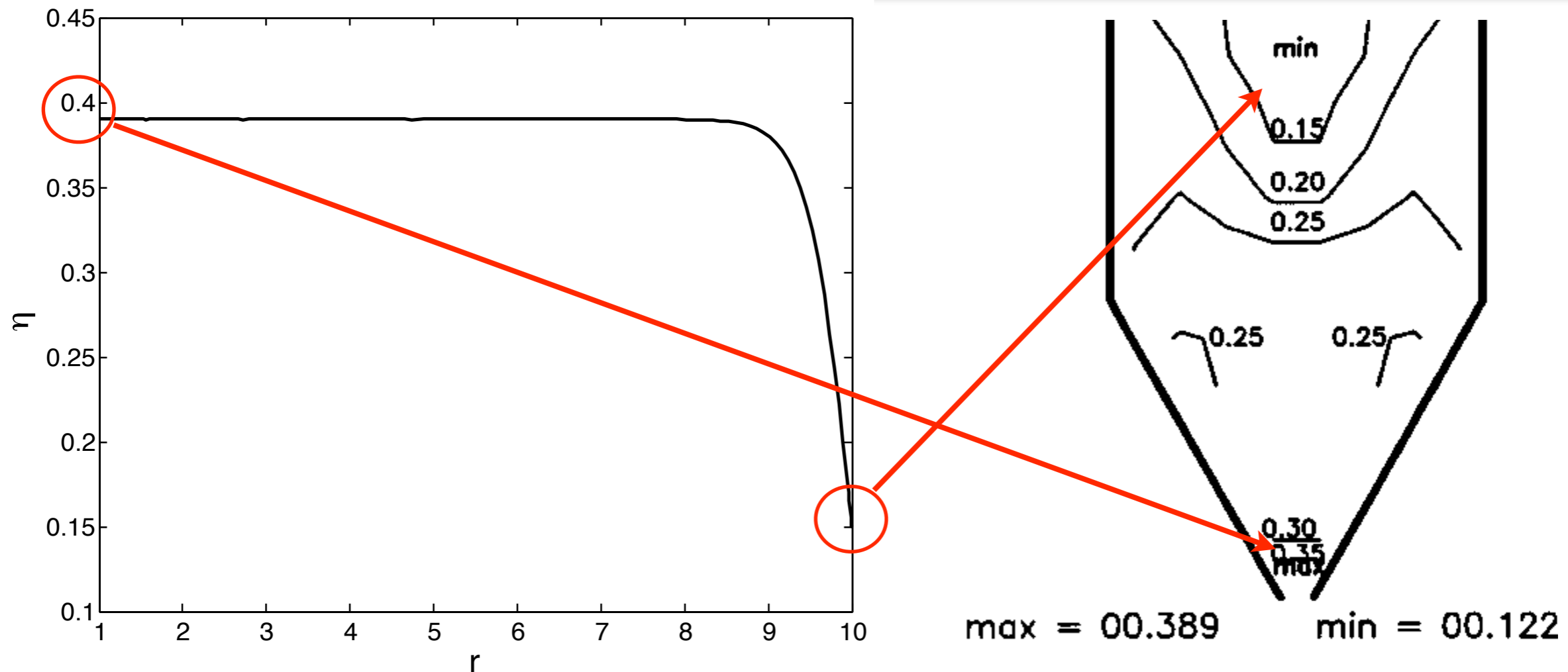
- Stress profile is similar to that of hour-glass theory.

# Predictions of stress and macroscopic friction



- Stress profile is similar to that of hour-glass theory.
- Normal stress difference affects the prediction.

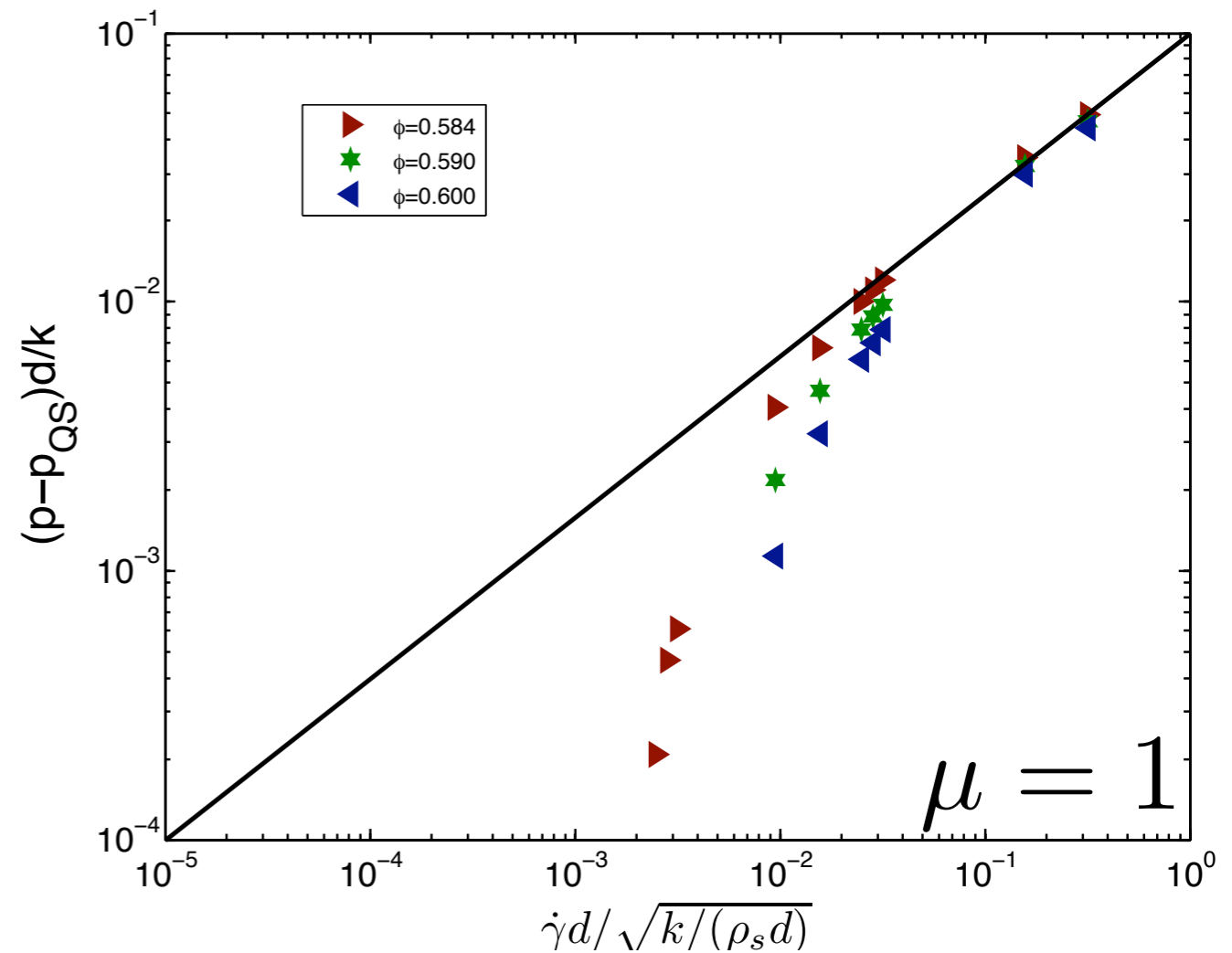
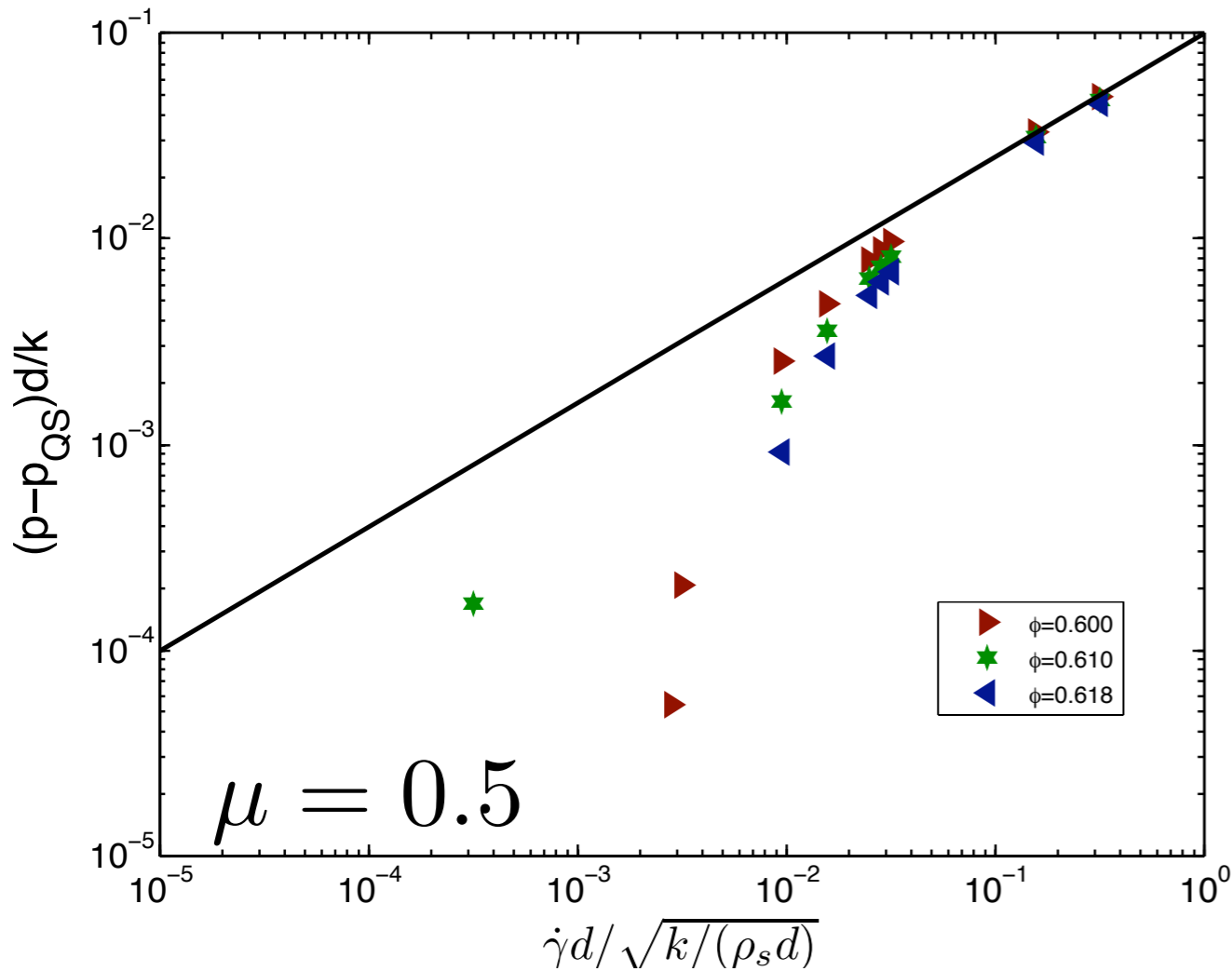
# Predictions of stress and macroscopic friction



- Stress profile is similar to that of hour-glass theory.
- Normal stress difference affects the prediction.
- Macro-friction varies in the flow direction and values agree with DEM simulations\*.

\*A.V. Potapov and C. S. Campbell. Physics of Fluids, 8(11):2884–2894, 11 1996.

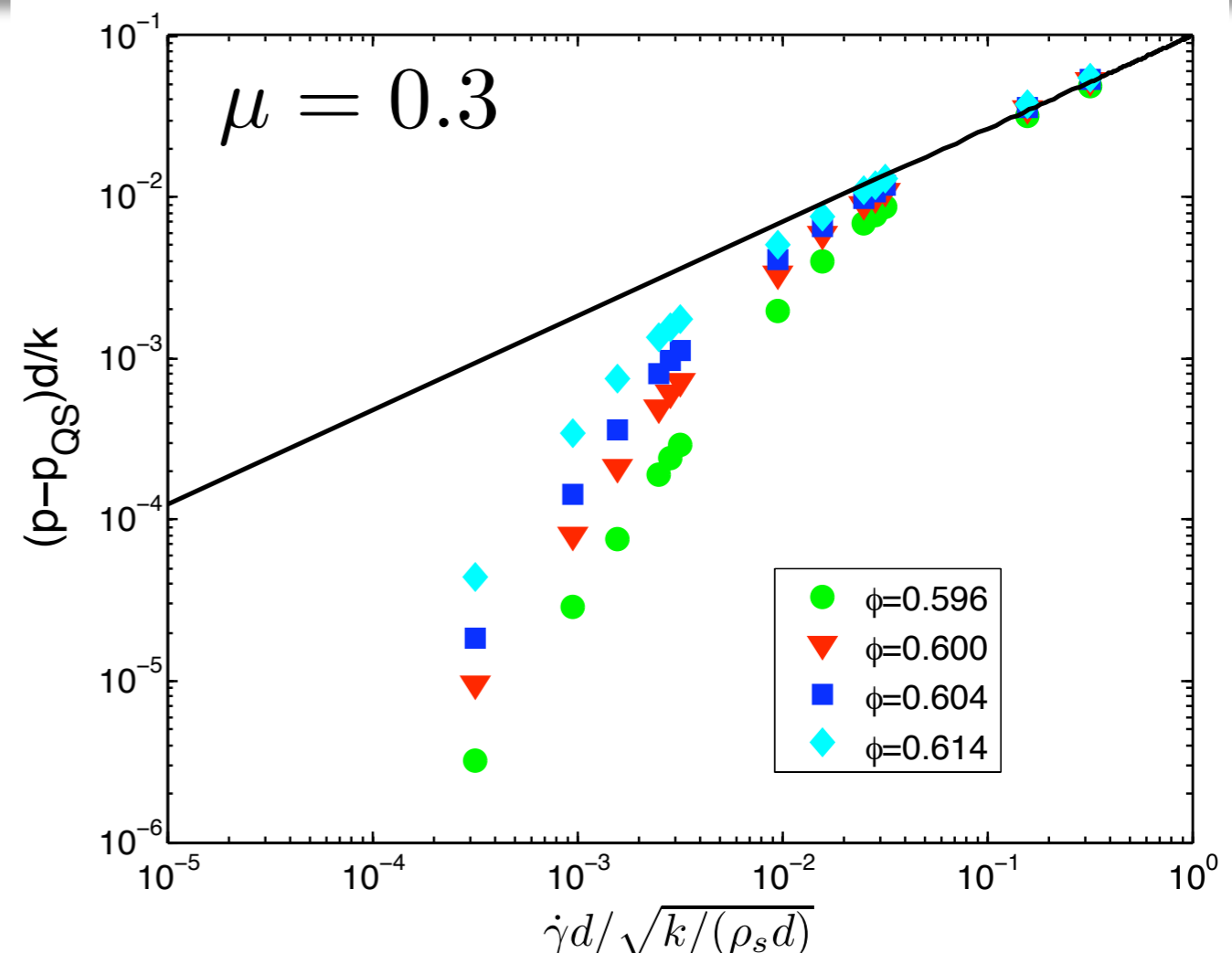
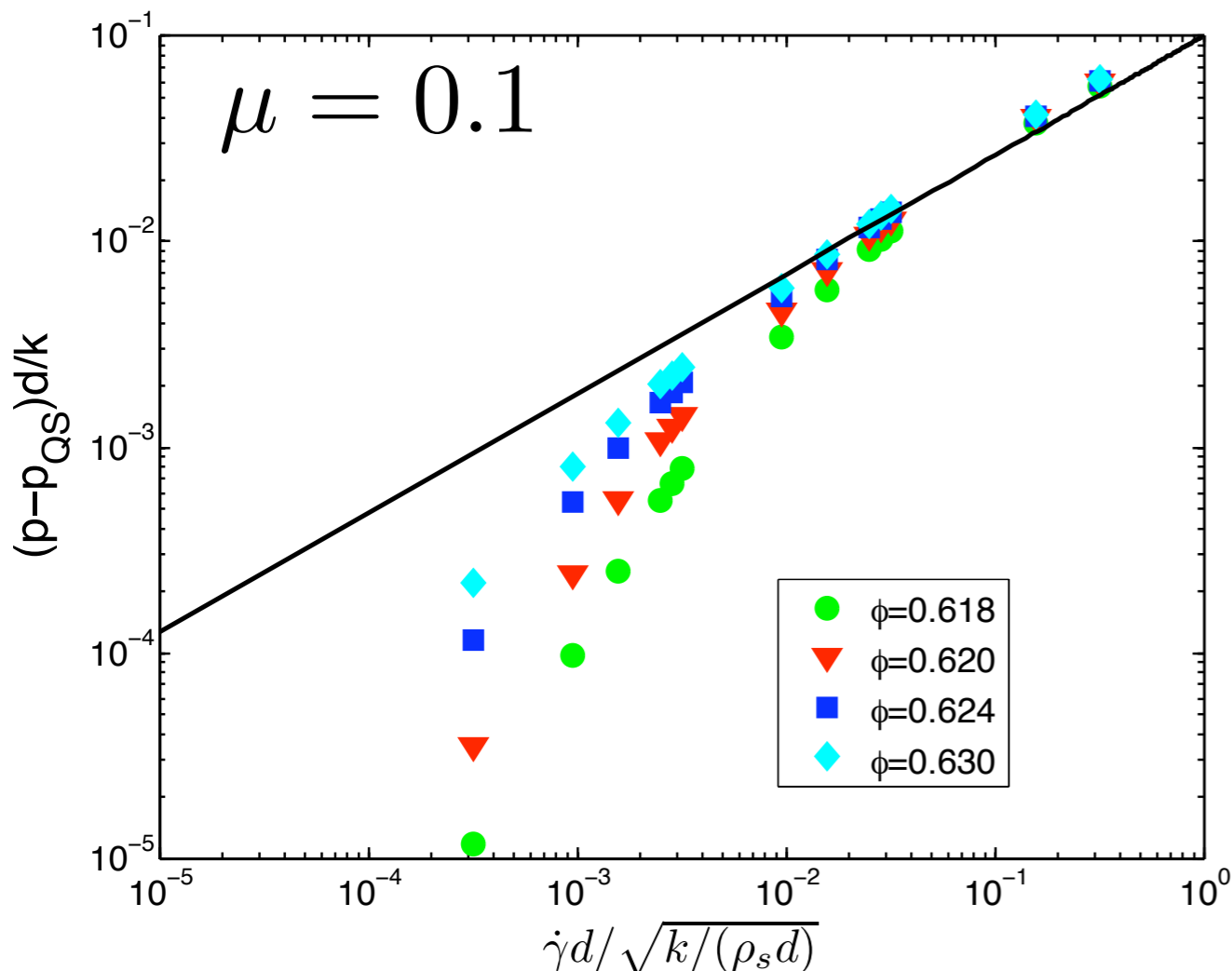
# Intermediate pressure behaviors



Collapse pressure data of assemblies with volume fractions  $\phi > \phi_c$  using  $(p - p_{QS})d/k = \alpha|\tilde{D}|^n$

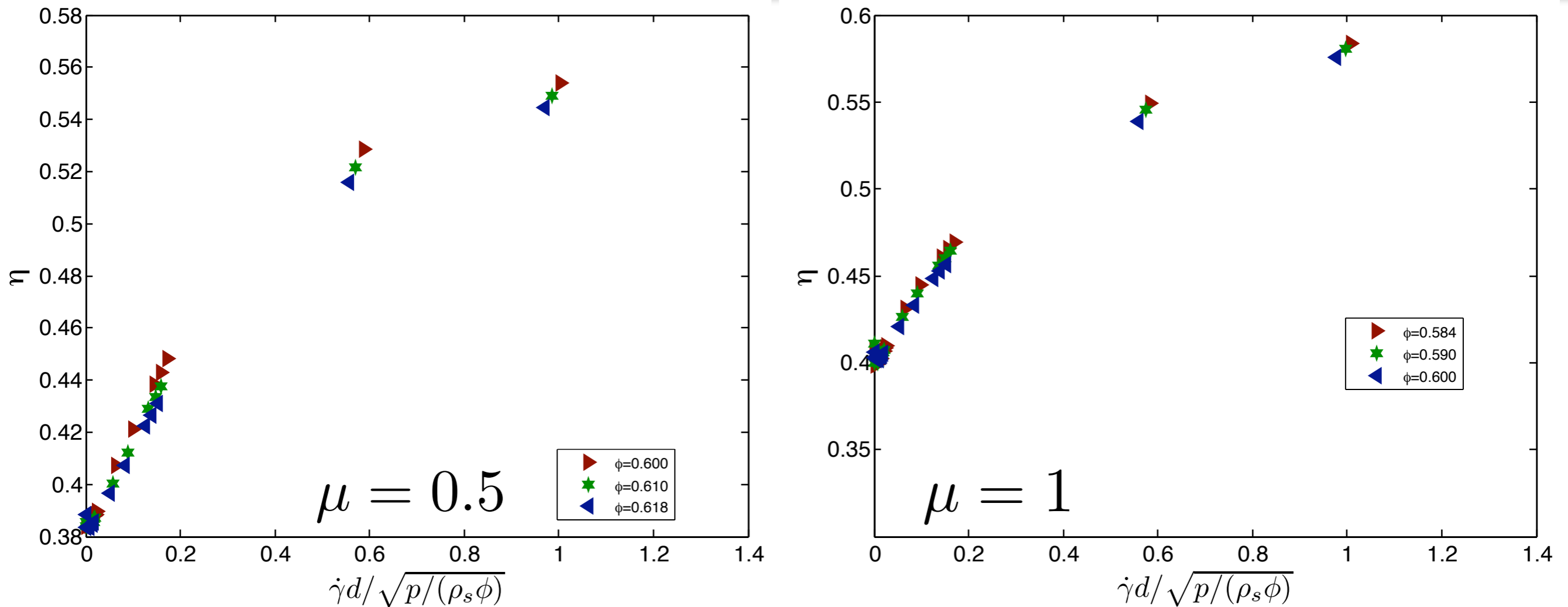
$p_{QS}$  is the pressure at the quasi-static state.

# Intermediate pressure behaviors



- Same relation works for a range of particle friction.
- Exponent  $n$  increases slightly with higher friction.

# Intermediate stress ratio

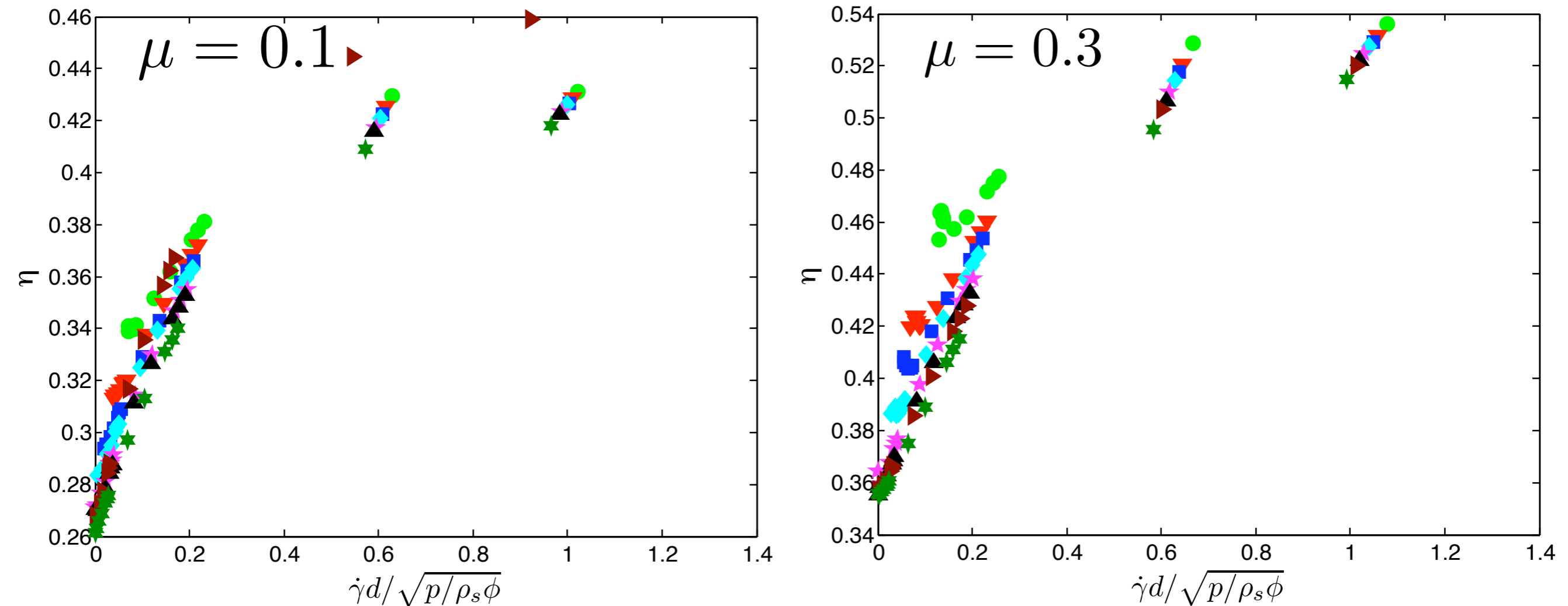


Macroscopic friction coefficients collapse onto one curve when plotted against inertia number\*

$$I = \dot{\gamma}d / \sqrt{p / \rho_s \phi}$$

\*P. Jop, Y. Forterre, and O. Pouliquen. *Nature*, 441 (7094):727–730, 2006.

# Intermediate stress ratio



- The collapse works for all the friction coefficient studied.
- The  $\eta$  scaling with  $I$  and correlation with friction are being examined.

# Work in progress



- Complete the model according to the flow behaviors shown for intermediate regime
- Extend the model to include rapid to intermediate flow transition
- Apply the model to compressible hopper flows

## Acknowledgment

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